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Synthesis, Characterization, and Structure of Tri-μ-halogeno-hexacarbonyldirhenate(I) Salts of Monocationic Porphyrin Acids.

by

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Synthesis, Characterization, and Structure of Tri-μ-halogeno-hexacarbonyldirhenate(I) Salts of Monocationic Porphyrin Acids

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ABSTRACT

Two new compounds, μ-[2,3,7,8,12,13,17,18-octaethylporphyrin]-bis-[tricarbonylrhenium(I)], $(C_{36}H_{44}N_4)[Re(CO)_3]_2$ and a salt of a monocationic porphyrin acid, octaethylporphinium tri-μ-chlorohexacarbonyldirhenate(I), $(C_{36}H_{47}N_4)^+[Re_2(CO)_6Cl_3]^-$, have been synthesized by the reaction of a 2:1 mole ratio of rhenium pentacarbonyl and octaethylporphyrin in refluxing decalin under argon. The structure of the latter was determined from three-dimensional diffractometer data. A total of 10,792 independent reflections was measured. The compound crystallizes in the monoclinic space group $P2_1/a$ with a unit cell of a = 18.140(3), b = 19.847(3), c = 13.625(2)A, β = 111.64(2)°. There are four molecules in the unit cell. The structure was solved by heavy-atom methods and refined by least-squares techniques to a conventional R index of 0.045 for the 5995 reflections having $I \geq 3\sigma_I$. The porphyrin monoacid cation has three coplanar pyrrole rings with the plane of the fourth ring tilted by 8.6° from the mean plane of the other three. Evidence indicates that the nitrogen atom in the tilted ring has sp^3 hybridization. The anion, which was hitherto unknown, consists of two rhenium atoms bridged by three chlorine atoms. Three carbonyl groups complete the octahedral coordination on each metal atom. There is a water molecule of crystallization which is involved in hydrogen bonding with the pyrrole nitrogen atoms of the cation. The salt could also be prepared using a 1.5/1 $Re(CO)_5Cl/H_2OEP$ mixture with $(H\text{-}OEP)Re(CO)_3$ as the other product. Analagous compounds could be made using mesoporphyrin IX dimethyl ester and $Re(CO)_5Br$, but the monocationic porphyrin species could not be ob-

tained when meso-tetraphenylporphyrin was used.

INTRODUCTION

The metal-carbonyl insertion method[2] has been found useful for the preparation of bimetallic porphyrin complexes of rhodium, rhenium, and technetium.[3-6] Metal carbonyl halides are more reactive reagents than metal carbonyls for the synthesis of bimetallic complexes of porphyrins as well as bimetallic salts of porphyrin acids.[6-8] For example, dimeric rhodium dicarbonyl chloride reacts with porphyrin in benzene at ambient temperature or in boiling chloroform to form a dirhodium porphyrin complex or a dirhodium salt of a porphyrin diacid.[9,10] In the present work it was discovered that dimeric rhenium tetracarbonyl halides are also capable of reacting with porphyrin in refluxing decalin to form a monorhenium or a dirhenium porphyrin complex as well as a salt complex of a porphyrin monoacid.[11] This salt contains a hitherto unreported anionic dimeric halocarbonyl rhenium complex, tri-μ-halogeno-hexacarbonyldirhenate(I). The structure of the salt containing chlorine as the halogen and octaethylporphinium monoacid as the cation has been elucidated by several means, primary among them being an x-ray structural analysis. A preliminary communication on this work has been published.[11]

Only a few porphyrin acid structures have been reported. Most of these have been porphyrin diacids. The earlier studies revealed macrocycles with large deviations from planarity, presumably because of the non-bonded interactions between the four imino hydrogen atoms.[7] However a more recent report on the structure of an H_4OEP^{2+} salt (OEP = octaethylporphyrin anion) showed that the macrocycle in that case was nearly planar.[10] Monoacid porphyrin cations are uncommon. Samuels, Shuttleworth, and Stevens[12] reported the preparation of a tri-iodo de-

rivative of octaethylporphyrin. A later x-ray structure determination, reported by Hirayama et. al. in a short communication, revealed that this compound should be formulated as $(H_3OEP)^+I_3^-$.[5] While the macrocycle in this case shows some deviations from planarity, the H-H contacts inside the porphyrin "hole" are still too short if the pyrrole nitrogen atoms are assumed to be trigonally hybridized. Thus partial sp^3 hybridization of the nitrogen atoms has been proposed for both the monocationic and dicationic octaethylporphyrin salts.[5,10] Such a hybridization would be necessary to explain the proposed hydrogen bonding in the H_4OEP^{2+} structure.[10]

In all of the porphyrin acid structures so far reported, the data have not been of sufficient quality to examine these suggestions adequately. However in the present case, crystals of excellent quality were available. Thus in addition to elucidating the nature of the material obtained in the synthetic procedure, a full x-ray analysis promised to shed some light on the nature and conformations of the porphyrin acids.

RESULTS AND DISCUSSION

Monocation Porphyrinium Tri-μ-halogeno-hexacarbonyldirhenate(I).

When a mixture of $Re(CO)_5Cl$ and H_2OEP in a 2:1 mole ratio was refluxed in decalin under argon and then allowed to stand at room temperature, a large quantity of burgundy colored crystals formed, leaving a solution of dirhenium octaethylporphyrin complex, $OEP[Re(CO)_3]_2$. The burgundy colored substance was recrystallized from dichloromethane/cyclohexane as dark red crystals, (I), mp 215-220°. The

structure of the new compound was formulated as $(H_3OEP)^+ [Re_2(CO)_6Cl_3]^-$, monocation octaethylporphinium tri-μ-chlorohexacarbonyldirhenate(I), based on elemental analysis, spectroscopic data, and a single-crystal x-ray diffraction analysis.

Compound I has visible absorptions in dichloromethane at 390 (Soret band), 530, 555, 570, and 602 nm. The visible spectrum is extremely similar to that of monocation octaethylporphinium triiodide, $(H_3OEP)^+ \cdot I_3^-$ (the only previously known porphyrin monocation salt)[5], and is distinctly different from that of the dication salt, $(H_4OEP)^{++} \cdot 2Cl^-$ (Figure I).[6] When ethanol is added to the dichloromethane solution of I, the visible spectrum reverts to that of metal free octaethylporphyrin H_2OEP. The infrared spectrum of I in the solid state (KBr pellet) has two broad peaks at 3350 and 3375 cm^{-1} attributed to stretching vibrations of the two chemically independent N-H bonds, and three strong metal-carbonyl stretching bands at 1950, 2020, and 2050 cm^{-1}. The far-infrared spectrum of I (in Nujol) has two broad metal-halide stretching peaks at 200 and 250 cm^{-1}. The pmr solution of I in deuteriochloroform shows two sharp peaks at 1.90 (t) and 4.20 (q) δ for the ethyl substituents and two broad peaks at 10.70 and -3.50 δ for the bridged methine protons and the pyrrolic N-H protons, respectively.

The new compound I is moisture sensitive and thermally unstable. It is fairly stable in dry methylene chloride, tetrahydrofuran, and ethylacetate but decomposes immediately in alcohols, acetone, and water to free octaethylporphyrin, H_2OEP. It can be kept under argon for several days without decomposition in a vacuum desiccator stored in a refrigerator. However, it decomposes gradually to dirhenium octaethyl-

porphyrin as indicated by its visible absorption spectrum. This behavior was confirmed by heating a purified sample of I in decalin under argon (Figure 2). Dirhenium octaethylporphyrin formed in the supernatant while the undecomposed burgundy colored solid of I remained at the bottom of the reaction flask. The amount of the dirhenium octaethylporphyrin varied with the heating time and temperature. Prolonged heating of I in refluxing decalin caused further decomposition to monorhenium octaethylporphyrin, $(H\text{-}OEP)Re(CO)_3$, as indicated by its visible absorption spectrum.[11]

By reaction of $H_2MPIXDME$ with stoichiometric quantities of $Re(CO)_5Br$ or $[Re(CO)_4Br]_2$ in refluxing decalin under argon, an analogous salt-like complex of I was prepared: $(H_3MPIXDME)^+[Re_2(CO)_6Br_3]^-$, (II), monocation mesoporphyrinium IX dimethyl ester tri-μ-bromo-hexacarbonyl dirhenate(I). This complex has chemical and spectroscopic properties similar to that of I (Figure 3). Therefore, a structure identical to that of I is proposed for II.

On the basis of the stepwise changes of visible absorption spectra of the reaction mixture and the x-ray crystal structure of I, the following reaction scheme was proposed.

$$H_2OEP + Re(CO)_5Cl \longrightarrow (H\text{-}OEP)Re(CO)_3 + HCl + 2CO\uparrow$$

$$(H\text{-}OEP)Re(CO)_3 + Re(CO)_5Cl \longrightarrow OEP[Re(CO)_3]_2 + HCl + 2CO\uparrow$$

$$2Re(CO)_5Cl \longrightarrow [Re(CO)_4Cl]_2 + 2CO\uparrow$$

$$[Re(CO)_4Cl]_2 + HCl \longrightarrow H^+[Re_2(CO)_6Cl_3]^- + 2CO\uparrow$$

$$H_2OEP + HCl \longrightarrow (H_3OEP)^+Cl^-$$

$$(H_3OEP)^+Cl^- + H^+[Re_2(CO)_6Cl_3]^- \longrightarrow (H_3OEP)^+[Re_2(CO)_6Cl_3]^- + HCl$$

$$2H_2OEP + 4Re(CO)_5Cl \longrightarrow (H_3OEP)^+[Re_2(CO)_6Cl_3]^- + OEP[Re(CO)_3]_2 + HCl\uparrow + 8CO\uparrow$$

Because of the instability of meso-tetraphenylporphine monocation,[6,7] none of the corresponding monocation tetraphenylporphinium analogues could be prepared; possible reasons for this instability are outlined by Fleischer.[6]

X-Ray Structural Data

A preliminary study on the single crystal x-ray diffraction analysis of (I) has already been reported.[11] It is an ionic compound with the porphyrin moiety present as a monocationic species, H_3OEP^+. In the anionic species $[Re_2(CO)_6Cl_3]^-$, the two rhenium ions have octahedral coordination. They are joined by three bridging chlorine atoms. Three carbonyl groups on each metal ion complete the coordination. ORTEP[13] drawings of the compound are shown in Figure 4. Figure 4a also shows the nomenclature for the different types of carbon atoms and the designations for the four rings. A stereoview of the entire formula unit, including a water molecule of crystallization, is shown in Figure 5.

A. Cation

The imino hydrogen atoms appear to be localized on Rings A, B, and C. Such a localization was postulated for the H_3OEP^+ cation as found in the tri-iodide salt.[5] The hydrogen atoms in that study were not located directly, but the C_a-N-C_a angle for one ring was reported as 102° as compared to the values of 109° and 110° for the other two crystallographically independent rings, which presumably bear imino hydrogen atoms. A similar difference is noted in the present case. Bond lengths and angles are tabulated in Table I. Some non-bonded con-

tacts of interest are also shown. Ring D, the pyrollenine ring, has a C_a-N-C_a bond angle of 105.3(6)°, while the analogous angles on the other three rings are 110.6(6)°, 108.3(6)°, and 110.8(6)°. These values correspond to those tabulated by Hoard[14] for pyrrole rings respectively lacking and carrying an N-H bond in free base porphyrins.

Unlike the earlier studies, electron density peaks corresponding to the imino hydrogen atoms were found in the present case, thus confirming the localization of the hydrogen atoms. No evidence of any electron density corresponding to a hydrogen atom bonded to N(4) (Ring D) was found.

Of particular interest is the planarity of the cation. The free base of octaethylporphyrin is essentially planar. The structure of meso-tetraphenylporphyrin, H_2TPP, has been reported as planar in a triclinic crystalline modifification[15] and as non-planar in a tetragonal crystalline modification.[16] Three structures of divalent cationic porphyrin species have been reported. In the two earlier studies, both of which involved meso-substituted porphyrins, the cations are decidedly non-planar.[7] In these non-planar species, the symmetry of the cations may be described as S_4. The non-planarity of these cations has been postulated as a mechanism for relieving the crowding of the imino hydrogen atoms. In a much more recent study, the H_4OEP^{2+} cation, as observed in a crystalline salt formulated as $(H_4OEP^{2+})[Rh(Cl_2)(CO)_2^-]_2$, is nearly planar.[10]

As in the earlier study,[5] the monovalent H_3OEP^+ cation in the present work has three of the four pyrrole rings (A,C,D) approximately coplanar. Information on least squares planes is given in Table II.

As is normally found the individual pyrrole rings are planar. For rings A, C, and D the interplanar angles between adjacent pyrrole rings are 3.2° and 2.7°. The maximum deviation of an atom from the mean plane of these three rings is 0.07Å (for C(2)). The fourth ring (B) is tilted by 8.6° from the plane of the other three rings. By way of comparison, this angle is 14° in the triiodide salt. In the current study, interplanar angles between Ring B and the adjacent rings are 7.9° and 9.8°.

It is believed that this deviation from planarity is due in part to the tight H-H contacts of the imino hydrogens. Ring B, the one which is not coplanar, bears the imino hydrogen atom which comes in closest contact with the other two imino hydrogen atoms. However this deviation from planarity is still not sufficient to relieve the tight contacts completely. In the present case, the H-H contacts are still ~ 1.5-1.6Å if we assume trigonal hybridization and a N-H bond length of 1.0Å. The minimum H-H non-bonded contact is usually taken to be 1.9-2.0Å.[17]

In both the H_4OEP^{2+} salt[10] and in the triiodide salt of H_3OEP^+,[5] sp^3 hybridization of the nitrogen atoms has been postulated. Such a hybridization would be advantageous for a number of reasons. Most importantly, such a hybridization would relieve the tight H-H contacts. A second reason would be to explain the hydrogen bonding arrangement found in some of these compounds.

In the case of the H_4OEP^{2+} salt,[10] hydrogen bonds are postulated between the pyrrole nitrogen atoms and one of the chlorine atoms of the anion. For this to occur, the N-H bonds need to point more or less directly towards the chlorine atoms, as would be the case if there were sp^3 hybridization of the nitrogen atoms.

In the triiodide salt of H_3OEP^+,[5], no hydrogen-bonding is reported. In the present case there is hydrogen bonding between the pyrrole nitrogen atoms and the water molecule of solvation. Intermolecular contacts between pyrrole nitrogen atoms and the oxygen atom of the water molecule are shown schematically in Figure 6. N...O distances are 2.97, 2.99 and 3.05Å for N(1), N(2) and N(4) respectively. These are short enough to be considered hydrogen bonding distances. The fourth N..O distance (N(3)...O(7)) is 3.22Å, probably too long to be considered a hydrogen bond. There are also fairly short intermolecular distances between the water molecule and two of the chlorine atoms of the anion (O(7)-Cl(1) 3.43Å; O(7)-Cl(2), 3.46Å) but these are probably too long to be considered O...Cl hydrogen bonds.

At least one of the hydrogen bonds should involve an imino hydrogen atom, especially since N(4) has no hydrogen atom of its own, and yet is implicated in the hydrogen bonding scheme. The observed hydrogen atom positions would indicate that N(2) has at least some degree of sp^3 hybridization, whereas N(1) and N(3) are trigonally hybridized. H(1) and H(3) are 0.13Å and 0.04Å respectively out of the planes defined by the pyrrole rings to which they are bonded. The bond angles also indicate trigonal hybridization. On the other hand H(2) is 0.67Å out of the plane of Ring B in the direction of the water molecule. The N(2)-H(2)..O(7) angle is 148°. The problem of tight H-H contacts is also eliminated. The three H-H contacts are now 2.62Å (H(1)-H(2)); 3.00 (H(1)-H(3)); and 2.34Å (H(2)-H(3)). If the hydrogen atom positions are given idealized values (assuming sp^3 hybridization for N(2), trigonal hybridization for N(1) and N(3), and a N-H bond length of 1.0Å) the corresponding H-H contacts are 2.22, 2.23 and 2.19Å.

A caveat should be observed here. The positions of hydrogen atoms are difficult to locate when heavy, highly scattering atoms such as rhenium and chlorine are present and the accuracy of these positions is quite low. The N-H observed bond lengths in this case are certainly underestimated and the angles involving H(2) differ considerably from ideal values. Thus the observed hydrogen atom positions should be viewed as merely an indication of the nature of the nitrogen atom hybridization. However, other supportive geometric evidence for the suggested hybridization is available.

The C_a-N-C_a angle in Ring B (108.3(6)°) is considerably less than that found in Rings A and C (110.6(6)° and 110.8(5)°). In an N-substituted porphyrin, ethoxycarbonylmethyloctaethylporphyrin,[18] the C_a-N-C_a angle is 107° on the pyrrole ring which has the substituent on the nitrogen atom. There is little doubt the nitrogen atom in this ring has sp^3 hybridization. On the other hand the angle is 110° in the ring in which the nitrogen atom is trigonally hybridized and bears a hydrogen atom.

The C_a-N bond lengths provide inconclusive evidence for this hybridization scheme. One would expect a bond length of ~ 1.41Å if sp^3 hybridization were present, as opposed to ~ 1.38Å if there were trigonal hybridization.[4,18] The C_a-N distances are slightly longer in Ring B than in the other rings, but this difference is not statistically significant. Given the e.s.d. of ~ 0.01Å in a bond length, it is not unexpected that a difference, if there is one, cannot be observed.

The average C_a-C_b distance of 1.42(1)Å is somewhat shorter than the usual 1.44Å, but once again it is difficult to judge the statistical significance of the difference. The C_b-C_b distances fall within

the range tabulated by Hoard.[14] With the exception of the C_a-C_m-C_a angles, other bond parameters in the macrocyclic skeleton agree well with those tabulated. These angles are larger than expected, especially those involving atoms in Ring B. Opening of the C_a-C_m-C_a angle would further increase the distance between the hydrogen atoms. In an oxo-dipyrromethene where both pyrrole rings bear imino hydrogen atoms, the angle is 133°, presumably to relieve the close H-H contacts.[19] Since Ring D does not bear an imino hydrogen atom, the need for an extension of the C_a-C_m-C_a angle is eliminated and the angles involving this ring are smaller.

The values for terminal C-C bonds are unusually short. This is a common observation for octaethylporphyrin complexes and is probably due to thermal shortening. Previous experience has shown that when these bond distances are corrected for thermal motion assuming a "riding" model, more reasonable values are obtained.[20] However, thermal shortening does not completely explain the short C(35)-C(36) distance. This is undoubtedly short because of the unusually long C(18)-C(35) distance. No explanation for this long bond length is readily available. The large thermal ellipsoids and standard deviations for C(35) and C(36) may indicate some disorder, but attempts to resolve this possible disorder failed. This bond length was long in separate refinements using both the copper and molybdenum radiation data (see experimental section).

B. Complex Anion

The preparative,[21-26] mechanistic[27,28] and spectroscopic[29-31] properties of halocarbonyls of rhenium(I) have been extensively studied in the past. Four series of halocarbonyl anions of rhenium(I) have been reported: $[Re(CO)_3X_3]^{2-}$, $[Re(CO)_4X_2]^-$, $[Re_2(CO)_7X_3]^-$, and $[Re_2(CO)_6X_4]^{2-}$.[32,33]

The structure of these anions were deduced from infrared spectroscopic data. To our knowledge anions of the type found in the present study, $[Re_2(CO)_6X_3]^-$, have not been previously reported. No structural data have been reported for these anionic rhenium(I) halocarbonyls. However the structure of a closely related neutral complex has been reported. In this compound one of the bridging chlorine atoms has been replaced by a bis(diphenylarsino)methane group (abbreviated as dam). In the anion in the present work the average Re-Cl distance is 2.51(1)Å, the average Re-C distance is 1.88(2)Å, while the average C-O distance is 1.15(2)Å. These numbers agree well with those found in $Re_2(CO)_6(dam)Cl_2$ as do many of the other bond parameters.[35] The Re-C and C-O distances also agree with those found in $TPP[Re(CO)_3]_2$.[4] The Re(1)-Re(2) distance of 3.375(1)Å is too long to postulate any sort of metal-metal interactions. None would be expected.

C. Molecular Packing

A stereoview of the packing in the unit cell is shown in Figure 7. The reason for all eight terminal carbon atoms being pointed in one direction with respect to the porphyrin ring is apparent from this figure. With this arrangement steric interactions with the porphyrin cation related by a center of symmetry are avoided. This was also observed in N-ethyoxycarbonylmethyl-octaethylporphyrin.[18] The interplanar separation between the cation and its centrosymmetrically related nearest neighbor is 3.4Å, which is the approximate layer separation in graphite. However there are no unusually close contacts between atoms in the two macrocycles. A listing of the intermolecular contacts $\leq$ 3.5Å are given in Table III.

With the obvious exception of the hydrogen bonding distances between the cation and the water molecule, and with the possible exception of the Cl(2)-O(7) and Cl(3)-O(7) distances which, though unlikely, may correspond to weak O...Cl hydrogen-bonding distances, none of these contacts is expected to have any significant effect on the observed structure.

EXPERIMENTAL SECTION

Materials

Octaethylporphyrin, H_2OEP, was purchased from Strem Chemical Co.; Dirhenium decacarbonyl, $Re_2(CO)_{10}$, and rhenium pentacarbonyl chloride, $Re(CO)_5Cl$, were purchased from Pressure Chemical Co.; Decahydronaphthalene (decalin) was purchased from J. T. Baker Chemical Co., treated with concentrated sulfuric acid, neutralized with sodium bicarbonate solution, washed with distilled water, dried over anhydrous calcium chloride overnight, filtered, and further dried over sodium wire; finally it was distilled under vacuum and stored in a Schlenk tube under argon before use. Other organic solvents were reagent grade chemicals, dried over type 4A molecular sieve and distilled under argon before use.

Rhenium pentacarbonyl bromide, $Re(CO)_5Br$, and dimeric rhenium tetracarbonyl bromide, $[Re(CO)_4Br]_2$, were prepared by literature procedures.[36-38]

Physical Measurements

Elemental analyses were performed by Schwarzkopf Microanalytical Laboratory, Woodside, New York, 11377. Visible spectra were measured with a Cary 14 spectrophotometer. Infrared spectra were measured with a Beckman IR-8 spectrophotometer. Mass spectra were obtained on a CEC-21-104 mass spectrometer. Proton Magnetic resonance spectra were ob-

tained using Varian T-60 spectrometers.

Monocation Octaethylporphirium Tri-μ-chlorohexacarbonyldirhenate(I), $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$, (I)

A mixture of 95 mg (0.26 mmol) $Re(CO)_5Cl$ and 65.5 mg (0.13 mmol) H_2OEP was refluxed in decalin under argon. The progress of the reaction was followed by visible spectroscopy. The reaction was complete after 20 hr of refluxing. The decalin solution was then allowed to stand at room temperature. A large quantity of burgundy colored crystals were collected by centrifugation and washed with decalin and n-pentane. Finally, the crude product was recrystallized from dichloromethane/cyclohexane to give 84 mg (0.07 mmol) dark red crystals, (I), mp. 215-220°. Anal. Calcd for $Re_2C_{42}H_{47}N_4O_6Cl_3$: Re, 31.50; N, 4.74; Cl, 8.98. Found: Re, 26.25; N, 4.81; Cl, 8.91. The supernatant contained only dirhenium octaethylporphyrin complex, $OEP[Re(CO)_3]_2$, as indicated by its visible spectrum. About 55 mg (0.05 mmol) of the dirhenium octaethylporphyrin complex was isolated from the supernatant solution.

The new complex I was also prepared by heating H_2OEP and $Re(CO)_5Cl$ in a 1:1.5 mole ratio in decalin under argon for approximately 5 hr. The supernatant contained only the monorhenium octaethylporphyrin complex, $(H\text{-}OEP)Re(CO)_3$, as indicated by its visible absorption spectrum. When equimolar quantities of H_2OEP and $Re(CO)_5Cl$ were refluxed in decalin under argon for approximately 3 hr, only the monorhenium octaethylporphyrin complex was formed.

Monocation Mesoporphyrinium IX Dimethyl Ester Tri-μ-bromohexacarbonyldirhenate(I), $(H_3MPIXDME)^+[Re_2(CO)_6Br_3]^-$ (II).

The reaction was carried out in essentially the same manner as that described above, with rhenium pentacarbonyl bromide, $Re(CO)_5Br$, substi-

tuted for $Re(CO)_5Cl$ as the metal source. A 120 mg sample of H_2MPIXDME (0.21 mmol) and 180 mg (0.44 mmol) of $Re(CO)_5Br$ in about 20 ml of decalin were heated under argon in an oil bath. The reaction was observed to proceed at a temperature of ca. 120° and the progress of the reaction was followed by visible absorption spectroscopy. A stepwise change in the absorption spectra (Figure 3) and a continuous change of color in the reaction mixture was observed. After 5 hr of heating, the decalin solution was cooled to room temperature. A large quantity of burgundy colored substance crystallized out and was collected by centrifugation, washed with decalin and n-pentane, and finally recrystallized from ethyl acetate/cyclohexane/dichloromethane to give 186 mg (0.14 mmol) dark red crystals, (II), mp 180-185°. Anal. Calcd for $Re_2C_{42}H_{43}N_4O_{10}Br_3$: C, 36.63; H, 3.13; Re, 27.10; N, 4.07; Br, 17.82. Found: C, 35.74; H, 3.26; Re, 29.74; N, 4.31; Br, 19.58. The supernatant contained only the dirhenium mesoporphyrin complex, MP$[Re(CO)_3]_2$, as indicated by its visible absorption spectrum. About 75 mg (0.067 mmol) of the dirhenium mesoporphyrin complex was isolated from the supernatant solution.

Compound <u>II</u> can also be prepared in essentially the same manner as that described above, with dimeric rhenium tetracarbonyl bromide, $[Re(CO)_4Br]_2$, substituted for $Re(CO)_5Br$ as the metal source. H_2MPIXDME (198 mg, 0.33 mmol) and $[Re(CO)_4Br]_2$ (304 mg, 0.40 mmol) were mixed in about 20 ml of decalin and heated under argon in an oil bath. The reaction was observed to proceed at a temperature of ca. 105° and the progress of the reaction was followed by visible absorption spectroscopy.

<u>Attempted Preparation of meso-Tetraphenylporphyrin Monocation Salt</u>

The reaction of stoichiometric quantities of $Re(CO)_5Cl$ with H_2TPP in

refluxing decalin under argon, in a manner similar to that used in preparing the salt-like complex I, resulted in a mixture of the meso-tetraphenylporphyrin dication salt, $(H_4TPP)^{++}\cdot 2Cl^-$, and the monorhenium tetraphenylporphyrin complex, $(H\text{-}TPP)Re(CO)_3$.

X-Ray Study

The crystals of I grew as parallelepipeds elongated along c and bounded by {110}. The crystal chosen for intensity measurements measured 0.23x0.34x0.44 mm. The crystal was mounted in a capillary at an arbitrary orientation,[39] but with the c axis approximately parallel to the spindle axis. In the capillary the crystal has remained stable for over two years.

Crystal data are listed in Table IV. Cell dimensions were determined by least squares, minimizing the differences between observed and calculated 2θ values. 24 Cu K_α (λ = 1.54178A) reflections, all having 2θ in the range 50-52.5°, were measured at both + and - 2θ. A Syntex-Datex automated diffractometer equipped with a graphite monochromator was used. The systematic absences uniquely determined the space group as $P2_1/a$.

A set of intensity data were collected on the Datex-Syntex diffractometer using Cu K_α radiation, using the θ-2θ method. A total of 4946 independent reflections were measured out to ca.100° in 2θ , the machine limit. Of these 3463 were considered observed and were used in the analysis. They were corrected for absorption effects using a Gaussian inegration method.

From these data the structure was elucidated, which provided the basis for the preliminary communication.[11] However for a number of reasons it was decided to recollect the data using Mo K_α radiation

(λ = 0.71069Å). At the machine limit of 100° in 2θ, a large percentage of the reflections still had intensities which were considered to be observed. Collection of the data to a higher sin θ/λ limit would increase the accuracy of the structural parameters. Also, the high linear absorption coefficient for Cu K_{α} radiation (119.5 cm^{-1}) introduces a large systematic error which an absorption correction could only approximately correct. Low order reflections are the most affected by absorption effects. It is these same reflections which contain a significant contribution from the scattering power of the hydrogen atoms. One of the hopes of this study was to locate the imino hydrogen atoms. In the presence of rhenium and chlorine atoms, which have a high scattering power, locating the hydrogen atoms would require a good set of data as free from systematic error as possible.

Therefore the data were recollected on a Syntex $P2_1$ diffractometer using Mo K_{α} radiation. The same crystal was used. Intensity data for 10,792 unique reflections, ($2\theta_{max}$ = 55°, (sin $\theta/\lambda)_{max}$ = 0.65) were obtained; the ω scan method was employed with a scan range of 0.6°. The scan rate varied from 2°/minute to 12°/minute, depending on the number of counts accumulated in a rapid preliminary scan. The intensities were normalized to counts/min. Background measurements were taken at both ends of the scan with ω displaced by 0.7° from the K_{α} peak; each measurement was made for one-half of the scan time. The intensities of the four standard reflections were monitored after every 89 reflections. Only statistical variations were observed and no corrections were applied.

Only the 5995 reflections with $I \geq 3\sigma_I$ were used in the analysis. The standard deviation σ_I was determined in terms of the statistical

variances of the counts as $\sigma_I^2 = \sigma_I^2$ (count) + $(0.03\ F_o)^2$ where F_o is the observed structure factor and σ_I^2(count) is the standard deviation based solely on counting statistics.

Absorption corrections were made to the data using a ψ scan technique, observing the change of intensity of the $52\bar{1}$ reflection. The minimum intensity observed for this reflection was 62% of the maximum. A scan of several other reflections gave similar results. Structure factors were calculated in the usual way assuming a 50% ideally perfect-50% ideally imperfect monochromator mounted in a parellel orientation.

<u>Determination and Refinement of the Structure</u>

Because there are four molecules in the unit cell of space group $P2_1/a$, no crystallographic symmetry is imposed on the molecule. The positions of the rhenium atoms were found from a Patterson synthesis, using the data collected with Cu K_α radiation. The positions of the remaining 56 non-hydrogen atoms were found from a series of difference Fourier maps. Included among these atoms was a peak attributable to a water molecule of crystallization.

Least-squares refinements using block diagonal and finally full-matrix methods were carried out. The function minimized was $\Sigma w(F_o-F_c)^2$ where $w = 1/\sigma_F^2$. Refinement using the Cu K_α data was not carried beyond the stage where isotropic temperature factors were used. At this stage $R = \Sigma\bigl||F_o|-|F_c|\bigr|/\Sigma F_o$ was 0·106.

Further refinement utilized the Mo K_α data. The thermal parameters of the non-hydrogen atoms were refined anisotropically. The large number of parameters required refining the formula unit in blocks, alternately refining the anion and then the cation and water molecule.

After several cycles of refinement, ΔF syntheses were calculated in an effort to locate hydrogen atoms. The three imino hydrogen atoms were thus found. However many of the hydrogens on the peripheral atoms were not located or were in chemically unreasonable positions. The positional parameters of the imino hydrogen atoms were refined. The thermal parameters for these three atoms were not refined, but were set as $B = 4.0\text{Å}^2$, as was the case for all hydrogen atoms. Idealized positions for the other hydrogen atoms were calculated except for those on the water molecule. A C-H bond length of 1.0Å and a staggered configuration for the methyl hydrogens was assumed. The contributions from these were added to the calculated structure factors but the positions were not refined. However, before the final cycles of refinement, new positions were calculated and used. The refinement converged with R = 0.046 and $R_w = \Sigma w\|F_o|-|F_c\|/\Sigma wF_o^2 =$ 0.047. The final value of the standard deviation of an observation of unit weight, defined as $|\Sigma w\|F_o|-|F_c\|^2/(N_o-N_v)|^{1/2}$ was 1.72 for $N_o = 5995$ reflections and $N_v = 532$ variables. In the last cycle of refinement all shifts were considerably less than one standard deviation. There were five peaks on the final difference Fourier which were above 1 e/Å^3. These were all close to the rhenium atoms. Neither they nor any other peak in the final difference Fourier were believed to have any physical significance.

Correction for anomalous dispersion were made for all non-hydrogen atoms.[40] Scattering factors were from Ref. 41. The rhenium and chlorine atoms were assumed to be in the zero ionization state. No evidence of secondary extinction was found.

The structure was solved and the initial refinement performed on

the IBM 360/65 and its successor at Texas A&M, the Amdahl 470 v/6. Most of the programs used have been listed elsewhere.[42,43] In addition the data collection and data reduction programs used for the molybdenum data are those supplied by Syntex Analytical Instruments. Most of the final refinements and calculations were performed on a PDP 11/40 computer using the Enraf-Nonius Structure Determination Package (SDP).

The final positional and thermal parameters for the nonhydrogen atoms and the three imino hydrogen atoms are given in Table V. The final calculated positions of the other hydrogen atoms are given in Table VI. Tables VII and VIII contain the root-mean-square-components of thermal displacement along the principal axes of the thermal ellipsoids and the observed and calculated structure factors respectively. Tables VI-VIII are available as supplementary material.

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Supplementary Material Available: Table VI-VIII containing the calculated lated hydrogen atom positions, the root-mean-square components along the principal axes of the thermal ellipsoids, and observed and calculated structure factors. Ordering information is given on any current masthead page.

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TABLE I

Bond Lengths (Å) and Angles (deg)[a]

A. Cation

N(1) -C(1)	1.377(9)	C(1) -N(1) -C(4)	110.6(6)
N(1) -C(4)	1.351(9)	C(6) -N(2) -C(9)	108.3(6)
N(2) -C(6)	1.382(8)	C(11)-N(3) -C(14)	110.8(5)
N(2) -C(9)	1.391(8)	C(16)-N(4) -C(19)	105.3(6)
N(3) -C(11)	1.378(8)	N(1) -C(1) -C(2)	106.4(6)
N(3) -C(14)	1.363(8)	N(1) -C(1) -C(20)	125.3(6)
N(4) -C(16)	1.367(8)	C(2) -C(1) -C(20)	128.2(6)
N(4) -C(19)	1.364(8)	C(1) -C(2) -C(3)	107.9(6)
C(1) -C(2)	1.406(9)	C(1) -C(2) -C(21)	124.6(7)
C(1) -C(20)	1.366(10)	C(3) -C(2) -C(21)	127.5(7)
C(2) -C(3)	1.381(9)	C(2) -C(3) -C(4)	107.7(6)
C(2) -C(21)	1.496(9)	C(2) -C(3) -C(23)	126.3(6)
C(3) -C(4)	1.407(9)	C(4) -C(3) -C(23)	126.0(6)
C(3) -C(23)	1.504(10)	N(1) -C(4) -C(3)	107.2(6)
C(4) -C(5)	1.391(9)	N(1) -C(4) -C(5)	124.6(6)
C(5) -C(6)	1.381(9)	C(3) -C(4) -C(5)	128.1(7)
C(6) -C(7)	1.417(9)	C(4) -C(5) -C(6)	131.3(6)
C(7) -C(8)	1.348(9)	N(2) -C(6) -C(5)	123.3(6)
C(7) -C(25)	1.523(10)	N(2) -C(6) -C(7)	107.4(6)
C(8) -C(9)	1.410(9)	C(5) -C(6) -C(7)	128.8(6)
C(8) -C(27)	1.516(9)	C(6) -C(7) -C(8)	108.2(6)
C(9) -C(10)	1.381(9)	C(6) -C(7) -C(25)	123.8(6)
C(10)-C(11)	1.352(9)	C(8) -C(7) -C(25)	128.0(6)
C(11)-C(12)	1.435(9)	C(7) -C(8) -C(9)	108.8(6)
C(12)-C(13)	1.358(9)	C(7) -C(8) -C(27)	127.6(6)
C(12)-C(29)	1.520(9)	C(9) -C(8) -C(27)	123.6(6)
C(13)-C(14)	1.421(8)	N(2) -C(9) -C(8)	107.1(6)
C(13)-C(31)	1.520(9)	N(2) -C(9) -C(10)	123.5(6)
C(14)-C(15)	1.392(9)	C(8) -C(9) -C(10)	129.2(6)
C(15)-C(16)	1.392(9)	C(9) -C(10)-C(11)	130.0(6)
C(16)-C(17)	1.425(9)	N(3) -C(11)-C(10)	125.6(6)
C(17)-C(18)	1.341(10)	N(3) -C(11)-C(12)	105.5(6)
C(17)-C(33)	1.495(10)	C(10)-C(11)-C(12)	129.0(6)
C(18)-C(19)	1.419(10)	C(11)-C(12)-C(13)	108.7(6)
C(18)-C(35)	1.698(20)	C(11)-C(12)-C(29)	123.3(6)
C(19)-C(20)	1.407(10)	C(13)-C(12)-C(29)	127.9(6)
C(21)-C(22)	1.458(13)	C(12)-C(13)-C(14)	107.9(6)
		C(12)-C(13)-C(31)	128.3(6)
C(23)-C(24)	1.467(12)	C(14)-C(13)-C31)	123.6(6)
		N(3) -C(14)-C(13)	107.1(6)
C(25)-C(26)	1.449(12)	N(3) -C(14)-C(15)	125.2(6)
		C(13)-C(14)-C(15)	127.7(6)
C(27)-C(28)	1.480(13)	C(14)-C(15)-C(16)	129.0(6)
		N(4) -C(16)-C(15)	124.1(6)
C(29)-C(30)	1.486(11)	N(4) -C(16)-C(17)	110.8(6)

C(31)-C(32)	1.472(10)
C(33)-C(34)	1.472(12)
C(35)-C(36)	1.262(18)
N(1) -H(1)	0.62(7)
N(2) -H(2)	0.84(7)
N(3) -H(3)	0.62(8)
N(1) -N(2)	3.002(9)
N(1) -N(4)	2.908(9)
N(2) -N(3)	2.940(9)
N(3) -N(4)	2.945(9)
N(1) -N(3)	4.226(8)
N(2) -N(4)	4.113(9)
C(5)-C(15)	6.782(10)
C(10)-C(20)	6.883(10)

C(15)-C(16)-C(17)	125.1(6)
C(16)-C(17)-C(18)	105.9(6)
C(16)-C(17)-C(33)	125.3(6)
C(18)-C(17)-C(33)	128.7(7)
C(17)-C(18)-C(19)	108.1(6)
C(17)-C(18)-C(35)	127.4(7)
C(19)-C(18)-C(35)	122.7(18)
N(4) -C(19)-C(18)	109.9(6)
N(4) -C(19)-C(20)	125.2(7)
C(18)-C(19)-C(20)	124.7(7)
C(1) -C(20)-C(19)	127.2(7)
C(2) -C(21)-C(22)	112.5(8)
C(3) -C(23)-C(24)	114.3(7)
C(7) -C(25)-C(26)	113.4(8)
C(8) -C(27)-C(28)	112.0(7)
C(12)-C(29)-C(30)	113.3(6)
C(13)-C(31)-C(32)	113.8(6)
C(17)-C(33)-C(34)	110.8(7)
C(18)-C(35)-C(36)	93.4(15)
C(1) -N(1) -H(1)	124 (8)
C(4) -N(1) -H(1)	124 (8)
C(6) -N(2) -H(2)	118 (5)
C(9) -N(2) -H(2)	98 (5)
C(11)-N(3)-H(3)	124 (9)
C(14)-N(3) H(3)	125 (9)

B. Anion

Re(1)-Cl(1)	2.517(2)
Re(1)-Cl(2)	2.501(2)
Re(1)-Cl(3)	2.493(2)
Re(1)-C(37)	1.889(8)
Re(1)-C(38)	1.852(10)
Re(1)-C(39)	1.877(8)
Re(2)-Cl(1)	2.530(2)
Re(2)-Cl(2)	2.509(2)
Re(2)-Cl(3)	2.501(2)
Re(2)-C(40)	1.091(9)
Re(2)-C(41)	1.897(9)
Re(2)-C(42)	1.867(9)
C(37)-0(1)	1.142(8)
C(38)-0(2)	1.191(9)
C(39)-0(3)	1.138(8)
C(40)-0(4)	1.158(9)
C(41)-0(5)	1.125(8)
C(41)-0(6)	1.159(9)
Re(1)-Re(2)	3.375(1)

Cl(1)-Re(1)-Cl(2)	79.06(5)
Cl(1)-Re(1)-Cl(3)	79.87(6)
Cl(1)-Re(1)-C(37)	171.0(2)
Cl(1)-Re(1)-C(38)	95.6(3)
Cl(1)-Re(1)-C(39)	97.1(2)
Cl(2)-Re(1)-C(37)	94.6(2)
Cl(2)-Re(1)-C(38)	93.8(2)
Cl(2)-Re(1)-C(39)	175.1(2)
Cl(3)-Re(1)-C(37)	92.9(2)
Cl(3)-Re(1)-C(38)	173.4(3)
Cl(3)-Re(1)-C(39)	95.7(2)
C(37)-Re(1)-C(38)	91.2(3)
C(37)-Re(1)-C(39)	88.9(3)
C(38)-Re(1)-C(39)	89.5(3)
Cl(1)-Re(2)-Cl(2)	76.68(5)
Cl(1)-Re(2)-Cl(3)	79.47(6)
Cl(1)-R3(2)-C(40)	96.57(2)
Cl(1)-Re(2)-C(41)	170.9(2)
Cl(1)-Re(2)-C(42)	97.5(3)
Cl(2)-Re(2)-Cl(3)	80.37(6)
Cl(2)-Re(2)-C(40)	174.8(2)
Cl(2)-Re(2)-C(41)	95.6(2)
Cl(2)-Re(2)-C(42)	93.9(3)

Cl(3)-Re(2)-C(40)	96.8(3)
Cl(3)-Re(2)-C(41)	92.7(2)
Cl(3)-Re(2)-C(42)	173.9(3)
C(40)-Re(2)-C(41)	88.9(3)
C(40)-Re(2)-C(42)	88.7(4)
C(41)-Re(2)-C(42)	89.9(3)
Re(1)-Cl(1)-Re(2)	83.93(6)
Re(1)-Cl(2)-Re(2)	84.70(6)
Re(1)-Cl(3)-Re(2)	85.02(6)
Re(1)-C(37)-O(1)	177.7(7)
Re(1)-C(38)-O(2)	177.8(8)
Re(1)-C(39)-O(3)	179.2(7)
Re(2)-C(40)-O(4)	179.1(8)
Re(2)-C(41)-O(5)	177.5(8)
Re(2)-C(42)-O(6)	178.7(8)

[a] Some nonbonded distances of interest are also given. Asterisks indicate corrections for thermal motion.

TABLE II

Least Squares Planes

A. Deviations (Å) From Planes

	Plane 1	Plane 2	Plane 3	Plane 4	Plane 5	Plane 6	Plane 7
N(1)	0.007	-0.027	-0.008	-0.003	-0.298	0.106	0.102
N(2)	0.127	0.027	0.092	0.208	-0.009	0.095	0.183
N(3)	-0.013	-0.027	-0.024	0.109	-0.504	-0.002	-0.016
N(4)	-0.024	0.027	-0.015	0.009	-0.677	0.117	0.013
C(1)	0.040	0.044	0.036	-0.008	-0.373	0.203	0.148
C(2)	0.102	0.082	0.091	0.016	-0.196	0.273	0.243
C(3)	0.050	-0.020	0.026	-0.018	-0.072	0.165	0.199
C(4)	0.035	-0.043	0.008	0.014	-0.094	0.105	0.154
C(5)	-0.107	-0.226	-0.147	-0.100	-0.111	-0.096	0.006
C(6)	0.002	-0.133	-0.042	0.057	0.018	-0.040	0.088
C(7)	-0.189	-0.371	-0.247	-0.105	-0.022	-0.295	-0.107
C(8)	-0.091	-0.266	-0.147	0.036	0.017	-0.225	-0.039
C(9)	0.078	-0.047	0.035	0.204	-0.005	-0.011	0.112
C(10)	0.094	-0.007	0.058	0.255	-0.108	-0.001	0.095
C(11)	0.052	0.001	0.030	0.213	-0.331	0.000	0.036
C(12)	0.060	0.034	0.045	0.258	-0.444	0.001	0.011
C(13)	0.009	0.024	0.000	0.183	-0.674	-0.002	-0.055
C(14)	-0.041	-0.009	-0.038	0.094	-0.708	0.002	-0.067
C(15)	-0.049	0.027	-0.035	0.054	-0.860	0.057	-0.071
C(16)	-0.023	0.064	-0.004	0.034	-0.830	0.130	-0.016
C(17)	0.004	0.139	0.036	0.033	-0.958	0.221	0.013
C(18)	-0.046	0.082	-0.016	-0.059	-0.946	0.198	-0.005
C(19)	-0.062	0.014	-0.046	-0.073	-0.771	0.135	-0.004
C(20)	-0.007	0.047	0.003	-0.055	-0.603	0.200	0.084
O(7)	2.254	2.228	2.241	2.304	1.844	2.311	2.304

B. Angles (deg) between Least-Squares Planes

	Plane 2	Plane 3	Plane 4	Plane 5	Plane 6	Plane 7
Plane 1	2.1	0.6	1.9	7.7	2.7	1.4
Plane 2		1.5	3.2	9.8	1.5	2.9
Plane 3			2.2	8.3	2.2	1.7
Plane 4				7.9	4.3	3.2
Plane 5					9.8	7.1
Plane 6						2.7

C. Equations of Planes[a]

Plane 1 Macrocycle: N(1)-N(4), C(1)-C(20)

$$11.711x + 12.286y - 8.909z = -2.725$$

Plane 2 N(1)-N(4)

$$11.992x + 11.703y - 9.197z = -2.854$$

Plane 3 N(1), N(3), N(4), C(1)-C(5), C(10)-C(20)

$$11.796x + 12.121y - 8.990z = -2.755$$

Plane 4 Ring A: N(1), C(1)-C(4)

$$11.274x + 12.454y - 9.063z = -2.909$$

Plane 5 Ring B: N(2), C(6)-C(9)

$$10.883x + 14.155y - 7.604z = -1.625$$

Plane 6 Ring C: N(3), C(11)-C(14)

$$12.296x + 11.627y - 9.032z = -2.812$$

Plane 7 Ring D: N(4), C(16)-C(19)

$$11.899x + 12.36y - 8.693z = -2.628$$

[a] All planes are unweighted. x, y, z are in monoclinic fractional coordinates.

TABLE III

Intermolecular Contacts (Å) ≤ 3.5Å

Cl(2)-O(7)	3.43	O(1) -C(33)[a]	3.47
Cl(3)-O(7)	3.47	O(1) -C(34)[a]	3.20
C(38)-O(7)	3.46	C(5) -C(31)[b]	3.45
N(1) -O(7)	2.97*	C(27)-C(33)[b]	3.47
N(2) -O(7)	2.99*	O(1) -C(24)[c]	3.30
N(3) -O(7)	3.22	O(2) -O(4)[d]	3.09
N(4) -O(7)	3.05*	O(3) -C(21)[e]	3.38
O(2) -C(10)	3.19		
O(2) -C(11)	3.24		
O(6) -C(36)	3.42		

Superscripts denote the following equivalent positions relative to positions given in Table V. No superscript indicates only the identity transformation has been made. Asterisks indicate hydrogen-bonding distances.

a $-x, -y, -z$

b $-x, -y, 1-z$

c $-\frac{1}{2}+x, \frac{1}{2}-y, -1+z$

d $-\frac{1}{2}+x, \frac{1}{2}-y, z$

e $\frac{1}{2}-x, \frac{1}{2}+y, -1+z$

TABLE IV

Crystal Data for $(C_{36}H_{47}N_4)^+[Re_2(CO)_6Cl_3]^- \cdot H_2O$[a]

a = 18.140(3)Å	F.W. = 1200.6
b = 19.847(3)Å	Z = 4
c = 13.625(2)Å	d_{calcd} = 1.75 g/cm^3
β = 111.64(2)	μ = 58.4 cm^{-1}(Mo K_α radiation)
V = 4559Å^3	

SYSTEMATIC ABSENCES: h0ℓ(h odd); 0k0(k odd)

SPACE GROUP: $P2_1/a$

a Estimated standard deviation of least significant figures shown in parentheses

Table V

Fractional Coordinates and Thermal Motion Parameters Derived from the Least-Squares Refinement[a]

[a]In this and subsequent tables estimated standard deviations for the least significant figure are in parentheses. The Debye-Waller factor is defined as $T=\exp[-2\pi^2(U_{11}a^{*2}h^2+U_{22}b^{*2}k^2+U_{33}c^{*2}l^2+U_{12}a^*b^*hk+U_{13}a^*c^*hl+U_{33}b^*c^*kl)]$.

The values for U have been multiplied by 10^3, except for those of Re which have been multiplied by 10^4. For those atoms refined isotropically, the values for B (multiplied by a factor of 10) are given in the column labeled U_{11}. Isotropic temperature factors are defined by $T=\exp[-B(\sin^2\theta)/\lambda^2]$.

ATOM	X	Y	Z	U(11)	U(22)	U(33)	U(12)	U(13)	U(23)
RE(1)	0.12959(1)	0.19521(1)	0.16057(2)	435(1)	517(1)	626(1)	-46(3)	299(2)	-21(3)
RE(2)	0.29168(2)	0.09642(1)	0.21983(2)	486(1)	524(1)	542(1)	21(3)	165(2)	-99(3)
CL(1)	0.2647(1)	0.2032(1)	0.3048(1)	51(1)	52(1)	57(1)	-17(1)	22(1)	-21(1)
CL(2)	0.1532(1)	0.0741(1)	0.2135(1)	56(1)	49(1)	61(1)	-19(1)	31(1)	-6(1)
CL(3)	0.2143(1)	0.1635(1)	0.0594(1)	56(1)	64(1)	52(1)	2(2)	35(1)	-2(2)
N(1)	0.2259(3)	0.0536(3)	0.6760(5)	37(3)	69(4)	60(4)	17(6)	-13(6)	-14(7)
N(2)	0.0901(3)	0.1398(3)	0.5897(4)	42(3)	85(4)	39(3)	15(6)	29(4)	-13(6)
N(3)	0.0159(3)	0.0529(3)	0.4024(4)	38(3)	64(4)	40(3)	-8(6)	5(5)	-7(6)
N(4)	0.1637(3)	-0.0275(3)	0.4853(5)	48(3)	43(3)	63(4)	9(6)	0(6)	-4(6)
C(1)	0.2888(4)	0.0103(4)	0.6951(6)	38(4)	63(5)	60(5)	18(8)	-8(7)	-7(8)
C(2)	0.3459(4)	0.0300(4)	0.7918(6)	32(3)	61(5)	65(5)	3(7)	4(7)	7(8)
C(3)	0.3164(4)	0.0831(4)	0.8307(6)	37(3)	56(4)	46(4)	-20(7)	-2(6)	-18(7)
C(4)	0.2412(4)	0.0987(4)	0.7552(6)	52(4)	59(5)	49(4)	6(8)	24(6)	-4(8)
C(5)	0.1802(4)	0.1490(4)	0.7598(6)	47(4)	75(5)	43(4)	12(8)	10(6)	-17(8)
C(6)	0.1155(4)	0.1676(4)	0.6889(6)	45(4)	76(5)	49(4)	28(8)	24(6)	-6(8)
C(7)	0.0603(4)	0.2144(4)	0.7029(6)	53(4)	78(5)	46(4)	33(8)	24(6)	-21(8)
C(8)	-0.0039(4)	0.2174(4)	0.6121(6)	47(4)	68(5)	57(4)	22(8)	30(6)	-10(8)
C(9)	0.0065(4)	0.1702(4)	0.5404(5)	35(3)	80(5)	49(4)	27(7)	26(6)	13(8)
C(10)	-0.0467(4)	0.1512(4)	0.4424(6)	34(3)	71(5)	44(4)	25(7)	10(6)	0(8)
C(11)	-0.0437(4)	0.0997(4)	0.3796(6)	35(3)	60(4)	52(4)	13(7)	20(6)	4(8)
C(12)	-0.1023(4)	0.0803(4)	0.2782(5)	34(3)	67(5)	44(4)	1(7)	15(6)	0(7)
C(13)	-0.0729(4)	0.0248(4)	0.2442(5)	34(3)	55(4)	46(3)	-10(7)	16(5)	4(7)
C(14)	0.0315(4)	0.0073(3)	0.3225(5)	33(3)	48(4)	45(3)	0(7)	14(6)	0(7)
C(15)	0.0523(4)	-0.0445(4)	0.3189(6)	48(4)	48(4)	51(4)	-13(7)	11(7)	1(7)
C(16)	0.1271(4)	-0.0607(3)	0.3919(6)	43(4)	42(4)	62(4)	0(7)	17(7)	-3(7)
C(17)	0.1761(5)	-0.1139(4)	0.3900(7)	52(4)	57(4)	77(5)	39(8)	-10(8)	-29(9)
C(18)	0.2404(5)	-0.1143(4)	0.4695(8)	65(5)	66(5)	111(7)	71(9)	-52(11)	-57(10)
C(19)	0.2328(5)	-0.0611(4)	0.5347(7)	60(5)	63(5)	78(6)	33(9)	-6(9)	-29(9)
C(20)	0.2916(5)	-0.0423(4)	0.6316(7)	49(4)	76(5)	81(6)	54(8)	-19(9)	-25(10)
C(21)	0.4271(5)	-0.0017(5)	0.8404(7)	52(5)	74(6)	90(6)	13(10)	-21(9)	-22(11)
C(22)	0.4862(6)	0.0320(7)	0.8082(13)	50(5)	110(9)	256(15)	28(13)	58(15)	-1(22)
C(23)	0.3572(5)	0.1192(5)	0.9736(7)	62(5)	97(7)	65(5)	41(10)	28(8)	7(10)
C(24)	0.3316(7)	0.1844(6)	0.9237(10)	89(6)	102(8)	115(9)	-36(14)	-17(15)	-24(15)
C(25)	0.0749(5)	0.2522(5)	0.8054(7)	55(5)	86(6)	75(5)	15(10)	22(8)	4(11)
C(26)	0.1275(6)	0.3095(6)	0.8207(9)	92(7)	92(7)	118(8)	11(13)	37(13)	[illegible](13)
C(27)	-0.0751(5)	0.2625([illegible])	0.5872(7)	61(5)	80(6)	68(5)	27(9)	24(8)	-24(9)
C(28)	-0.0636(7)	0.3285(6)	0.5443(9)	91(7)	102(7)	102(8)	69(13)	-12(14)	9(14)
C(29)	-0.1749(4)	0.1205(5)	0.2196(6)	33(3)	95(6)	60(4)	24(8)	7(7)	-29(9)
C(30)	-0.1644(5)	0.1702(5)	0.1441(8)	67(5)	90(6)	90(6)	74(10)	38(9)	57(11)
C(31)	-0.1094(5)	-0.0116(4)	0.1401(6)	41(4)	63(5)	63(4)	-15(8)	8(7)	1(9)
C(32)	-0.0744(5)	0.0068(5)	0.0620(6)	83(5)	82(6)	61(5)	-38(10)	37(8)	-43(10)
C(33)	0.1596(5)	-0.1551(4)	0.2825(8)	61(5)	63(5)	83(6)	20(9)	-7(10)	-23(10)
C(34)	0.19[illegible](6)	-0.1190(5)	0.3052(8)	63(6)	99(6)	103(7)	23(11)	4(11)	-66(12)
C(35)	0.3073(8)	-0.1776(8)	0.5156(9)	163(10)	217(13)	91(7)	-190(19)	58(14)	-39(18)
C(36)	0.3570(10)	-0.1500(7)	0.4839(11)	246(15)	115(11)	134(9)	4(22)	170(17)	17(17)
C(37)	0.0347(4)	0.1783(4)	0.0446(6)	54(4)	67(5)	70(5)	-3(8)	31(7)	14(9)
C(38)	0.0735(5)	0.2119(4)	0.2474(7)	95(6)	53(5)	69(5)	-59(9)	29(9)	-1(9)
C(39)	0.1205(4)	0.2866(4)	0.1224(7)	45(3)	58(5)	103(5)	25(8)	62(7)	-7(9)
C(40)	0.3062(5)	0.1217(4)	0.2252(7)	55(5)	60(5)	98(6)	9(9)	22(5)	-34(10)
C(41)	0.2064(4)	0.0201(4)	0.1386(7)	49(4)	59(5)	83(5)	-11(8)	7(8)	-28(9)
C(42)	0.3400(6)	0.3469(4)	0.3435(9)	76(6)	56(5)	89(6)	-14(10)	8(13)	-9(10)
O(1)	-0.0212(3)	0.1670(3)	-0.0272(6)	61(4)	107(5)	107(5)	-34(8)	-36(9)	18(9)
O(2)	0.0356(3)	0.2237(3)	0.7005(5)	103(3)	108(5)	118(4)	3(7)	142(5)	-5(8)
O(3)	0.1156(3)	0.3419(3)	0.0987(5)	103(4)	53(3)	154(5)	32(7)	87(8)	25(8)
O(4)	0.4561(3)	0.1377(4)	0.2273(6)	55(3)	113(5)	163(6)	-44(7)	69(7)	-54(10)
O(5)	0.2993(3)	-0.0237(3)	0.0877(5)	85(4)	73(4)	121(4)	1(7)	52(6)	-82(7)
O(6)	0.3707(5)	0.0150(4)	0.4191(6)	140(7)	99(5)	104(5)	28(11)	-36(10)	61(9)
O(7)	0.1883(3)	0.1236(3)	0.4706(4)	79(3)	79(4)	31(3)	-2(6)	73(5)	0(6)
H(1)	0.193 (3)	0.049 (3)	0.642 (4)	40					
H(2)	0.100 (3)	0.140 (3)	0.544 (4)	40					
H(3)	0.046 (3)	0.052 (3)	0.445 (4)	40					

CAPTIONS FOR FIGURES

Figure 1. Visible Spectra of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$ and $(H_4OEP)^{++}2Cl^-$.

Figure 2. Thermal Decomposition of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$ to Form $OEP[Re(CO)_3]_2$ in Refluxing Decalin.

Figure 3. Repeated Sean Spectrophotometry Showing Progress of the Formation of $(H\text{-}MP)Re(CO)_3$, $MP[Re(CO_3)]_2$ and $(H_3MPIXDME)^+[Re_2(CO)_6Br_3]^-$.

Figure 4. a. ORTEP[13] drawing of the porphyrin cation, H_3OEP^+. Numbering scheme is shown. Shown in parentheses are the designations for the various types of carbon atoms. The thermal ellipsoids are drawn for 50% probability, except those of the hydrogen atoms which are not drawn to scale. H(21) and H(40) are hidden behind C(26) and C(34) respectively.

b. ORTEP Drawing of the complex anion.

Figure 5. A stereoview of the formula unit of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^- \cdot H_2O$. The water of crystallization is illustrated by a large circle. Imino hydrogen atoms are indicated by small circles. Other hydrogen atoms have been omitted. The notation of the pyrrole rings is shown. Note the tilt of Ring B with respect to the macrocycle.

Figure 6. Schematic drawing showing the significant contacts between the porphyrins cation and the oxygen atom of the water of crystallization. The lines between nitrogen atoms signify the planes of the macrocycle. Of the hydrogen atoms shown, it is believed that only H(2) is involved in hydrogen-bonding. This is indicated by a solid line between H(2) and O(7). The N(2)-H(2)-O(7) bond angle is also shown.

Figure 7. Steroview of the packing in the unit cell. Circles of increasing size represent rhenium, chlorine and oxygen atoms respectively.

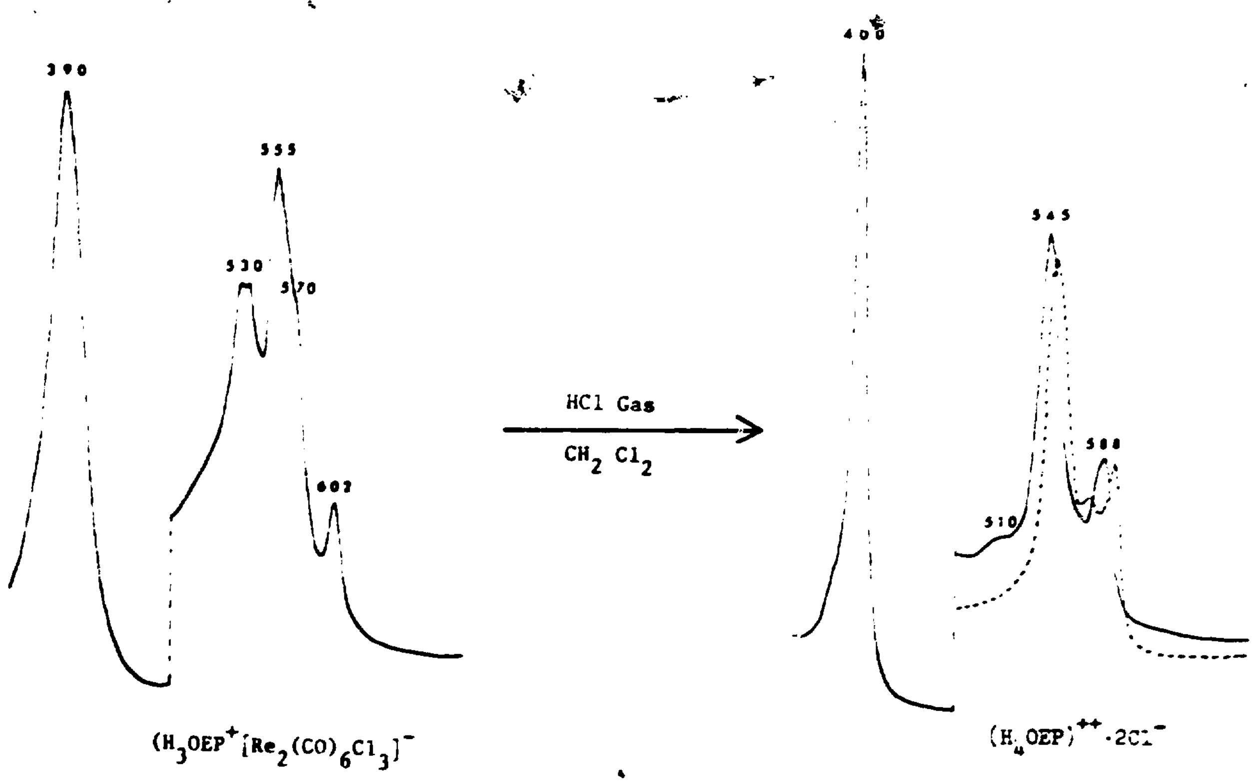

Figure 1. Visible Spectra of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$ and $(H_4OEP)^{++}2Cl^-$.

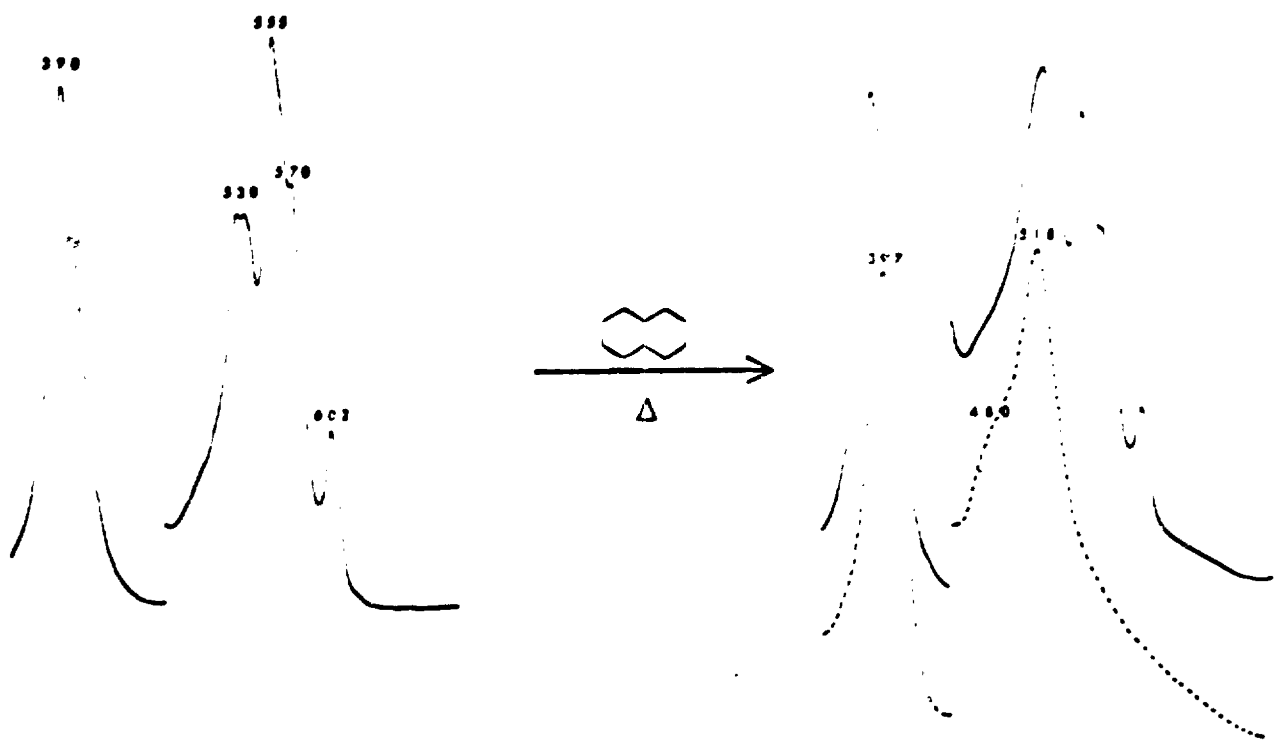

Figure 2. Thermal Decomposition of $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$ to Form $OEP[Re(CO)_3]_2$ in Refluxing Decalin.

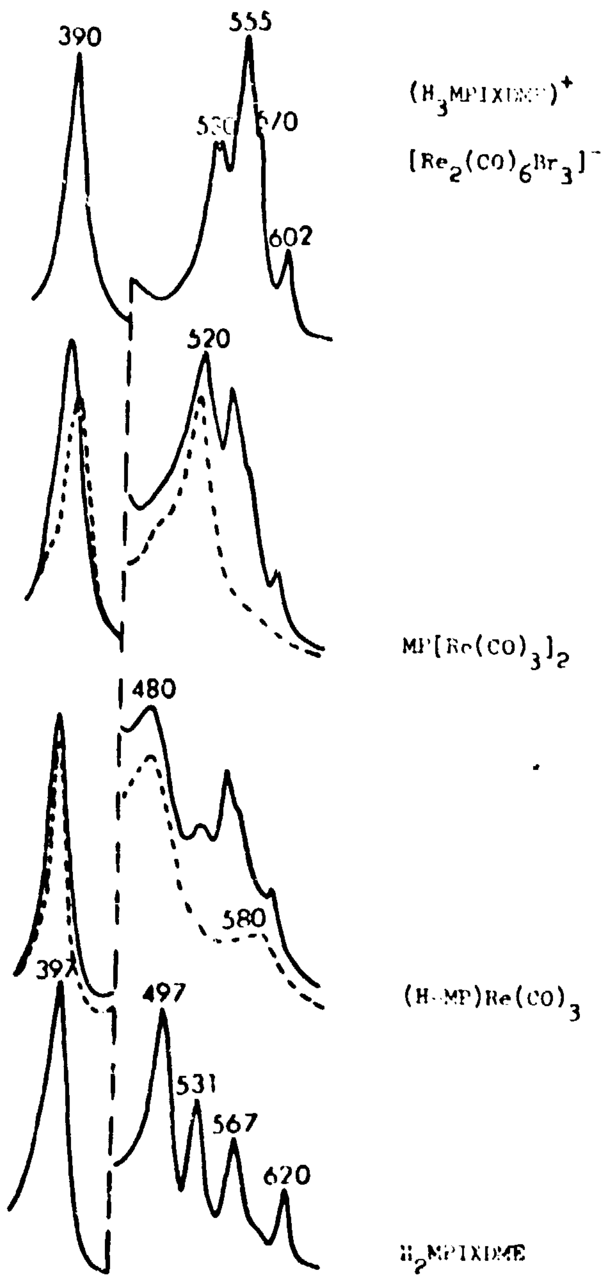

Figure 3. Repeated Scan Spectrophotometry Showing Progress of the Formation of $(H\text{-}MP)Re(CO)_3$, $MP[Re(CO)_3]_2$, and $(H_3MPIXDME)^+[Re(CO)_6Br_3]^-$.

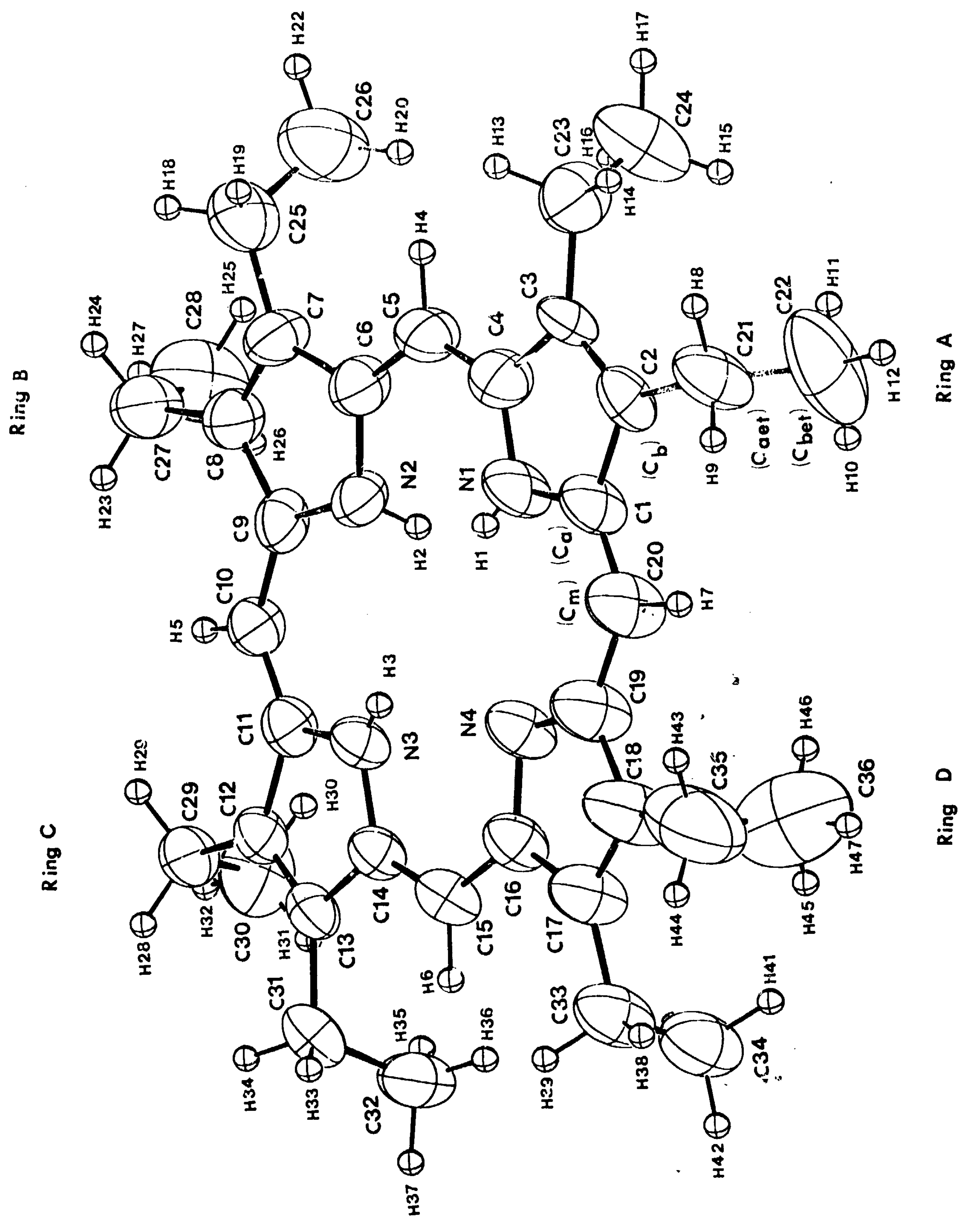
Ring A
Ring B
Ring C
Ring D
N1
N2
N3
N4
(Ca)
(Cb)
(Cm)
(Caet)
(Cbet)
C1
C2
C3
C4
C5
C6
C7
C8
C9
C10
C11
C12
C13
C14
C15
C16
C17
C18
C19
C20
C21
C22
C23
C24
C25
C26
C27
C28
C29
C30
C31
C32
C33
C34
C35
C36

Figure 4A

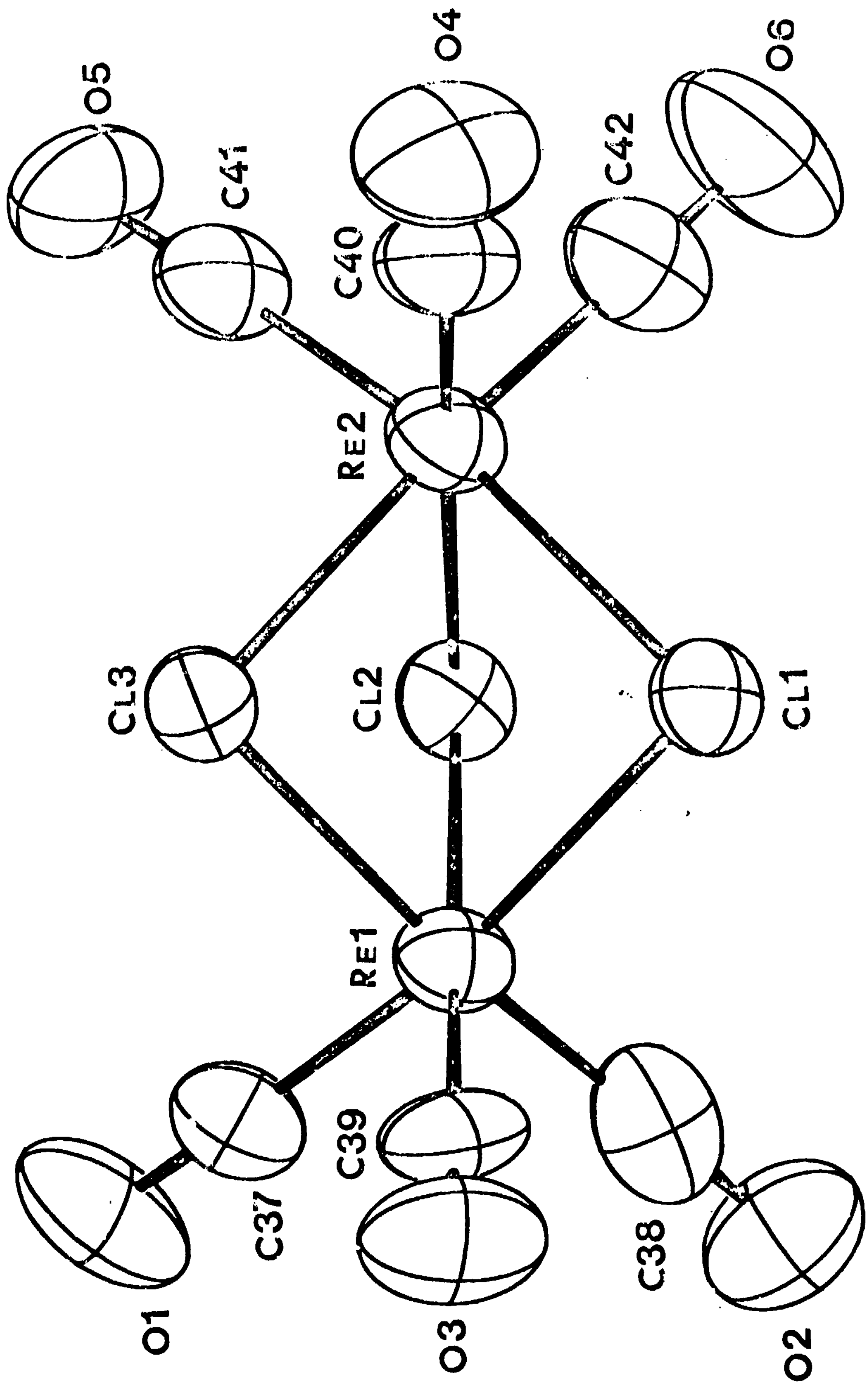

Figure 4B

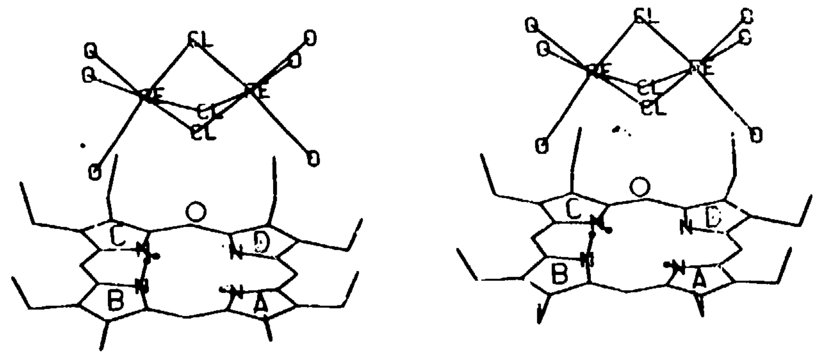

Figure 5

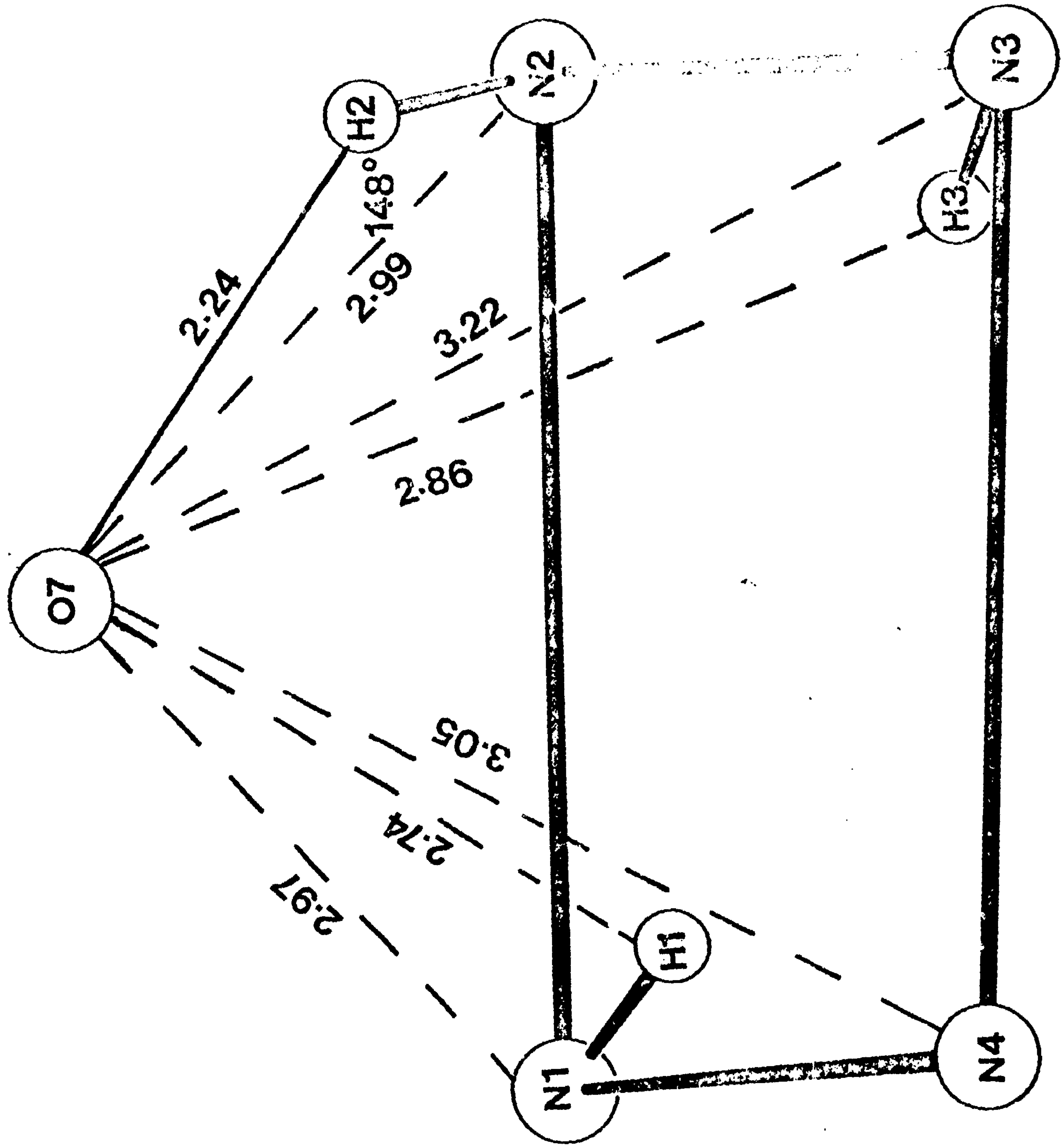

Figure 6

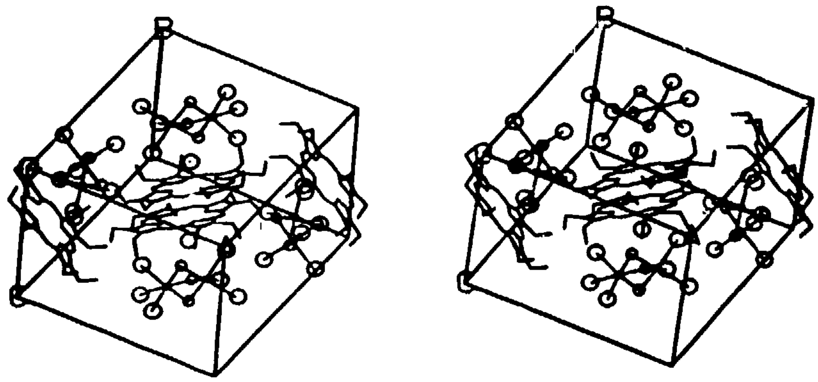

Figure 7

SUPPLEMENTARY MATERIAL

Synthesis, Characterization, and Structure of Tri-μ-halogeno-hexacarbonyldirhenate(I) Salts of Monocationic Porphyrin Acids

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SUPPLEMENTARY MATERIAL

TABLE VI

Calculated Hydrogen Atom Positions

ATOM	X	Y	Z	ATOM	X	Y	Z
H(4)	0.2085	0.1764	0.8261	H(25)	-0.0170	0.3521	0.5971
H(5)	-0.0949	0.1803	0.4134	H(26)	-0.0534	0.3213	0.4776
H(6)	0.0323	-0.0741	0.2552	H(27)	-0.1121	0.3566	0.5290
H(7)	0.3407	-0.0706	0.6568	H(28)	-0.2180	0.0886	0.1792
H(8)	0.4251	0.0020	0.9189	H(29)	-0.1909	0.1456	0.2722
H(9)	0.4241	-0.0496	0.8190	H(30)	-0.1220	0.2032	0.1826
H(10)	0.4704	0.0287	0.7294	H(31)	-0.1490	0.1462	0.0897
H(11)	0.4914	0.0803	0.8294	H(32)	-0.2154	0.1951	0.1076
H(12)	0.5393	0.0092	0.8425	H(33)	-0.1024	-0.0613	0.1535
H(13)	0.3[illegible]9	0.1272	0.9678	H(34)	-0.1675	-0.0009	0.1096
H(14)	[illegible]011	0.0898	0.9801	H(35)	-0.0818	0.0561	0.0470
H(15)	0.4322	0.1777	0.8903	H(36)	-0.0167	-0.0043	0.0909
H(16)	0.3491	0.2150	0.8780	H(37)	-0.1014	-0.0191	-0.0046
H(17)	0.4179	0.2051	0.9949	H(38)	0.1902	-0.1984	0.3017
H(18)	0.0226	0.2690	0.8048	H(39)	0.1018	-0.1653	0.2501
H(19)	0.0986	0.2207	0.8652	H(40)	0.1538	-0.0757	0.1852
H(20)	0.1802	0.2939	0.8223	H(41)	0.2422	-0.1088	0.2368
H(21)	0.1041	0.3421	0.7610	H(42)	0.1729	-0.1473	0.1496
H(22)	0.1340	0.3323	0.8888	H(43)	0.3257	-0.1812	0.5936
H(23)	-0.1217	0.2397	0.5341	H(44)	0.2862	-0.2207	0.4811
H(24)	-0.0853	0.2705	0.6536	H(45)	0.3349	-0.1451	0.4054
				H(46)	0.3744	-0.1057	0.5179
				H(47)	0.4052	-0.1810	0.5036

[a] All hydrogen atoms were assumed to have an isotropic thermal parameter, B = 4.0A^2

TABLE VII

ROOT-MEAN-SQUARE AMPLITUDES OF THERMAL VIBRATION IN ANGSTROMS.

ATOM	MIN.	INT'MED.	MAX.
N1	0.167	0.250	0.313
N2	0.194	0.204	0.299
N3	0.174	0.241	0.256
N4	0.193	0.209	0.301
C1	0.173	0.247	0.304
C2	0.174	0.248	0.286
C3	0.157	0.247	0.264
C4	0.215	0.243	0.268
C5	0.193	0.237	0.290
C6	0.199	0.224	0.293
C7	0.205	0.212	0.309
C8	0.204	0.234	0.281
C9	0.177	0.224	0.290
C10	0.170	0.229	0.280
C11	0.183	0.242	0.250
C12	0.182	0.229	0.260
C13	0.181	0.222	0.246
C14	0.187	0.219	0.236
C15	0.197	0.220	0.268
C16	0.206	0.213	0.275
C17	0.186	0.227	0.356
C18	0.172	0.237	0.456
C19	0.210	0.234	0.358
C20	0.172	0.257	0.374
C21	0.195	0.265	0.360
C22	0.217	0.337	0.529
C23	0.225	0.272	0.330
C24	0.242	0.333	0.422
C25	0.227	0.293	0.303
C26	0.275	0.298	0.396
C27	0.232	0.246	0.324
C28	0.227	0.327	0.417
C29	0.172	0.245	0.332
C30	0.192	0.314	0.350
C31	0.191	0.252	0.287
C32	0.214	0.293	0.320
C33	0.218	0.242	0.358
C34	0.239	0.254	0.401
C35	0.272	0.326	0.543
C36	0.330	0.356	0.496
O7	0.263	0.282	0.293

ATOM	MIN.	INT'MED.	MAX.
RE1	0.207	0.229	0.258
RE2	0.212	0.227	0.283
CL1	0.195	0.246	0.264
CL2	0.205	0.245	0.265
CL3	0.228	0.241	0.255
C37	0.232	0.250	0.288
C38	0.196	0.263	0.356
C39	0.185	0.272	0.325
C40	0.228	0.234	0.348
C41	0.201	0.249	0.328
C42	0.227	0.261	0.354
O1	0.204	0.319	0.419
O2	0.249	0.330	0.367
O3	0.220	0.327	0.399
O4	0.219	0.334	0.424
O5	0.221	0.292	0.395
O6	0.233	0.342	0.476

TABLE VIII

Values of 10 |Fo| and 10 |Fc|

For $(H_3OEP)^+[Re_2(CO)_6Cl_3]^-$

A. Data having $2\theta \leq 45°$

B. Data having $45° < 2\theta \leq 55°$

H3DEP+ REZ(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC PAGE 1

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
0	-18	0	753	730	11	-13	0	611	597	2	-8	0	261	238	10	-5	0	419	342	13	-2	0	1970	1885
1	-18	0	769	793	1	-12	0	2159	2114	3	-8	0	749	711	11	-5	0	1355	1281	15	-2	0	694	669
3	-18	0	769	759	2	-12	0	422	428	4	-8	0	1749	1701	13	-5	0	378	839	16	-2	0	888	849
4	-18	0	878	894	3	-12	0	186	155	6	-8	0	382	331	14	-5	0	351	307	1	-1	0	1797	1527
5	-18	0	295	329	4	-12	0	969	914	7	-8	0	229	170	15	-5	0	1617	1569	2	-1	0	2526	2113
2	-17	0	1158	1129	5	-12	0	732	691	8	-8	0	2376	2178	0	-4	0	1923	1871	3	-1	0	1203	1130
3	-17	0	273	234	7	-12	0	000	746	9	-8	0	382	353	1	-4	0	537	505	4	-1	0	959	880
4	-17	0	619	627	8	-12	0	967	953	10	-8	0	846	769	2	-4	0	3117	2888	5	-1	0	2062	1962
5	-17	0	1062	1063	9	-12	0	421	388	11	-8	0	809	738	3	-4	0	2951	2699	6	-1	0	3806	3558
6	-17	0	244	286	10	-12	0	838	775	12	-8	0	988	896	4	-4	0	1192	1077	7	-1	0	2517	2359
7	-17	0	685	637	11	-12	0	1287	1250	13	-8	0	1187	1114	5	-4	0	286	259	8	-1	0	1025	975
0	-16	0	380	374	1	-11	0	288	282	14	-8	0	368	304	6	-4	0	592	559	9	-1	0	979	961
1	-16	0	566	542	2	-11	0	338	363	1	-7	0	1383	1315	7	-4	0	2148	1938	10	-1	0	1276	1209
2	-16	0	797	778	3	-11	0	369	340	2	-7	0	2938	2792	8	-4	0	1309	1199	12	-1	0	345	344
3	-16	0	500	535	4	-11	0	1081	1012	4	-7	0	2468	2287	9	-4	0	1875	1737	13	-1	0	418	371
4	-16	0	1270	1237	5	-11	0	2065	1937	5	-7	0	2336	2149	10	-4	0	1037	950	14	-1	0	671	879
5	-16	0	584	590	6	-11	0	1928	1796	6	-7	0	543	479	12	-4	0	875	801	15	-1	0	482	435
7	-16	0	374	409	7	-11	0	2379	2251	7	-7	0	2291	2109	13	-4	0	644	625	16	-1	0	321	296
8	-16	0	1048	995	8	-11	0	721	706	8	-7	0	1459	1393	15	-4	0	888	877	2	0	0	3509	3214
1	-15	0	996	1012	9	-11	0	369	296	10	-7	0	1992	1867	1	-3	0	2094	1970	4	0	0	1694	1588
2	-15	0	417	413	10	-11	0	512	458	11	-7	0	1011	964	2	-3	0	4372	4061	6	0	0	798	750
3	-15	0	1649	1619	11	-11	0	730	393	13	-7	0	267	212	3	-3	0	1946	1732	8	0	0	740	743
4	-15	0	357	336	0	-10	0	3368	3401	14	-7	0	1257	1208	4	-3	0	1602	1466	10	0	0	911	919
5	-15	0	226	174	1	-10	0	1084	1011	15	-7	0	319	346	5	-3	0	449	336	12	0	0	2601	2498
9	-15	0	772	759	2	-10	0	1956	1855	0	-6	0	1197	1200	6	-3	0	1304	1198	14	0	0	1562	1455
10	-15	0	523	477	3	-10	0	494	495	1	-6	0	980	986	7	-3	0	1625	1550	16	0	0	346	321
0	-14	0	682	643	4	-10	0	691	638	2	-6	0	2087	1960	8	-3	0	970	935	0	-19	1	1145	1146
2	-14	0	745	720	5	-10	0	556	511	3	-6	0	1891	1789	9	-3	0	343	294	-5	-18	1	894	941
3	-14	0	1613	1599	8	-10	0	936	869	4	-6	0	2090	1934	10	-3	0	1411	1366	-4	-18	1	432	458
4	-14	0	362	360	10	-10	0	577	568	5	-6	0	1451	1376	11	-3	0	857	818	-3	-18	1	763	738
5	-14	0	1107	1057	12	-10	0	1694	1629	6	-6	0	236	233	13	-3	0	474	458	-2	-18	1	609	613
6	-14	0	217	84	13	-10	0	414	454	7	-6	0	1077	1012	14	-3	0	1341	1281	-1	-18	1	465	430
7	-14	0	855	822	1	-9	0	606	562	8	-6	0	1628	1436	15	-3	0	799	771	0	-18	1	459	435
8	-14	0	327	307	2	-9	0	1753	1689	9	-6	0	2382	2235	16	-3	0	728	665	2	-18	1	546	553
9	-14	0	1434	1369	3	-9	0	1298	1235	10	-6	0	817	774	0	-2	0	491	516	3	-18	1	596	573
10	-14	0	425	444	4	-9	0	1097	1006	11	-6	0	288	296	1	-2	0	5003	4614	4	-18	1	227	227
11	-14	0	298	333	5	-9	0	1581	1492	14	-6	0	319	316	2	-2	0	1787	1582	-6	-17	1	501	526
1	-13	0	611	610	6	-9	0	3326	3167	15	-6	0	464	466	3	-2	0	953	856	-4	-17	1	820	822
2	-13	0	1260	1225	7	-9	0	1157	1093	1	-5	0	2511	2364	4	-2	0	2326	2132	-3	-17	1	425	445
3	-13	0	784	739	8	-9	0	2226	2122	2	-5	0	945	888	5	-2	0	213	178	-1	-17	1	898	900
4	-13	0	1020	981	9	-9	0	1010	976	3	-5	0	1758	1726	6	-2	0	662	586	0	-17	1	243	210
5	-13	0	931	898	10	-9	0	598	579	4	-5	0	813	723	7	-2	0	353	350	1	-17	1	835	804
6	-13	0	969	924	11	-9	0	572	552	5	-5	0	580	553	8	-2	0	2163	2007	2	-17	1	950	939
7	-13	0	825	765	12	-9	0	618	562	6	-5	0	478	432	9	-2	0	223	194	3	-17	1	283	276
8	-13	0	680	641	14	-9	0	472	444	7	-5	0	253	194	10	-2	0	967	894	4	-17	1	1148	1112
9	-13	0	236	227	0	-8	0	2057	2018	8	-5	0	878	796	11	-2	0	1813	1765	5	-17	1	289	228
10	-13	0	340	342	1	-8	0	2927	2918	9	-5	0	2031	1910	12	-2	0	692	626	-7	-16	1	439	434

H3OEP+ REZ(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-6	-16	1	436	442	5	-14	1	485	502	-7	-11	1	354	325	-7	-9	1	411	449	13	-8	1	306	248
-5	-16	1	212	276	6	-14	1	521	488	-6	-11	1	472	492	-6	-9	1	1252	1284	14	-8	1	830	817
-4	-16	1	1330	1423	8	-14	1	329	270	-5	-11	1	850	872	-5	-9	1	489	498	-15	-7	1	384	407
-3	-16	1	1205	1279	9	-14	1	1409	1362	-4	-11	1	615	633	-4	-9	1	1128	1120	-13	-7	1	903	957
-2	-16	1	1442	1445	-12	-13	1	668	659	-3	-11	1	1036	1054	-3	-9	1	707	730	-12	-7	1	801	853
-1	-16	1	530	526	-10	-13	1	1088	1129	-2	-11	1	974	1006	-2	-9	1	2460	2469	-11	-7	1	265	299
1	-16	1	677	683	-9	-13	1	754	783	-1	-11	1	2775	2749	-1	-9	1	1162	1116	-10	-7	1	1935	2057
2	-16	1	680	659	-8	-13	1	956	962	0	-11	1	1884	1828	0	-9	1	3825	3762	-9	-7	1	437	441
3	-16	1	328	342	-7	-13	1	268	206	1	-11	1	1398	1373	1	-9	1	1533	1564	-8	-7	1	1782	1821
4	-16	1	301	309	-5	-13	1	1090	1144	3	-11	1	535	561	2	-9	1	887	892	-7	-7	1	216	211
5	-16	1	533	552	-4	-13	1	605	632	4	-11	1	574	548	3	-9	1	1557	1495	-6	-7	1	258	291
6	-16	1	252	221	-3	-13	1	451	455	6	-11	1	1145	1120	4	-9	1	796	781	-5	-7	1	1373	1424
7	-16	1	283	270	-2	-13	1	867	942	7	-11	1	657	667	5	-9	1	1357	1302	-4	-7	1	892	956
8	-16	1	811	743	-1	-13	1	1405	1390	8	-11	1	1008	981	6	-9	1	802	757	-3	-7	1	234	238
-10	-15	1	230	233	0	-13	1	773	755	9	-11	1	275	245	7	-9	1	356	383	-2	-7	1	587	561
-9	-15	1	1436	1489	1	-13	1	612	623	10	-11	1	605	598	8	-9	1	1149	1086	-1	-7	1	2750	2695
-8	-15	1	336	350	2	-13	1	1076	1068	11	-11	1	1416	1334	9	-9	1	679	699	0	-7	1	469	466
-7	-15	1	271	302	3	-13	1	934	922	12	-11	1	828	809	10	-9	1	846	818	1	-7	1	2257	2152
-6	-15	1	359	406	4	-13	1	1068	1027	-13	-10	1	273	267	11	-9	1	845	829	2	-7	1	2682	2564
-5	-15	1	1105	1120	6	-13	1	229	187	-12	-10	1	747	779	12	-9	1	1588	1479	3	-7	1	961	870
-4	-15	1	476	525	7	-13	1	1221	1199	-11	-10	1	416	409	13	-9	1	440	418	4	-7	1	2736	2613
-3	-15	1	689	727	8	-13	1	834	754	-8	-10	1	1823	1879	-15	-8	1	277	304	6	-7	1	511	442
-1	-15	1	298	293	10	-13	1	649	614	-7	-10	1	813	820	-14	-8	1	692	687	7	-7	1	930	851
0	-15	1	224	193	11	-13	1	838	767	-6	-10	1	2458	2627	-12	-8	1	653	692	8	-7	1	1413	1334
1	-15	1	498	491	-13	-12	1	251	189	-5	-10	1	535	542	-11	-8	1	270	303	9	-7	1	687	643
2	-15	1	427	390	-11	-12	1	696	691	-4	-10	1	250	256	-10	-8	1	688	692	10	-7	1	668	591
3	-15	1	1777	1774	-10	-12	1	492	515	-3	-10	1	570	578	-9	-8	1	1109	1170	11	-7	1	860	807
4	-15	1	459	442	-9	-12	1	519	536	-2	-10	1	468	474	-8	-8	1	1164	1195	13	-7	1	899	817
5	-15	1	695	677	-7	-12	1	1833	1894	-1	-10	1	227	234	-7	-8	1	2237	2307	14	-7	1	747	768
7	-15	1	1115	1038	-5	-12	1	1307	1348	0	-10	1	1595	1569	-6	-8	1	890	949	-15	-6	1	1084	1135
8	-15	1	371	371	-4	-12	1	1121	1185	1	-10	1	1095	1037	-5	-8	1	2003	2093	-14	-6	1	685	698
9	-15	1	1063	1010	-3	-12	1	359	377	2	-10	1	525	529	-4	-8	1	1163	1253	-13	-6	1	219	202
-11	-14	1	588	619	-2	-12	1	1362	1373	3	-10	1	567	525	-3	-8	1	160	139	-12	-6	1	575	583
-9	-14	1	281	311	0	-12	1	431	441	4	-10	1	2371	2205	-2	-8	1	2210	2259	-11	-6	1	885	916
-8	-14	1	403	424	1	-12	1	1303	1292	5	-10	1	661	645	-1	-8	1	163	135	-10	-6	1	1156	1184
-7	-14	1	719	711	2	-12	1	523	532	6	-10	1	2847	2673	0	-8	1	1081	1040	-9	-6	1	341	371
-6	-14	1	531	545	3	-12	1	590	575	7	-10	1	597	554	1	-8	1	919	865	-8	-6	1	1018	1015
-5	-14	1	673	656	4	-12	1	334	337	8	-10	1	923	848	2	-8	1	2389	2275	-7	-6	1	1052	1069
-4	-14	1	801	849	5	-12	1	2205	2113	12	-10	1	482	489	3	-8	1	1014	963	-6	-6	1	844	873
-3	-14	1	2138	2209	7	-12	1	1618	1456	13	-10	1	356	322	4	-8	1	1136	1061	-5	-6	1	985	1013
-2	-14	1	544	553	8	-12	1	859	854	-14	-9	1	1110	1195	5	-8	1	2882	2742	-4	-6	1	1620	1699
-1	-14	1	605	625	10	-12	1	841	790	-13	-9	1	362	420	6	-8	1	1632	1531	-3	-6	1	2601	2745
0	-14	1	247	221	12	-12	1	291	261	-12	-9	1	1086	1118	7	-8	1	2005	1886	-2	-6	1	1396	1405
1	-14	1	931	889	-13	-11	1	1160	1204	-11	-9	1	955	975	9	-8	1	886	811	-1	-6	1	1739	1766
2	-14	1	339	346	-12	-11	1	812	863	-10	-9	1	390	400	10	-8	1	1131	1048	0	-6	1	1266	1205
3	-14	1	574	569	-11	-11	1	553	619	-9	-9	1	602	622	11	-8	1	330	311	1	-6	1	2786	2594
4	-14	1	532	490	-8	-11	1	308	312	-8	-9	1	468	485	12	-8	1	274	308	2	-6	1	1178	1109

H3OEP+ RE2(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
3	-6	1	1062	955	-1	-4	1	1019	1085	-13	-2	1	984	980	6	-1	1	1070	1028	2	-16	2	1314	1289
4	-6	1	1150	1055	1	-4	1	1915	1766	-12	-2	1	753	754	8	-1	1	1202	1168	3	-16	2	717	706
5	-6	1	1439	1335	2	-4	1	954	881	-11	-2	1	797	765	10	-1	1	1050	1027	4	-16	2	1129	1118
6	-6	1	1545	1347	3	-4	1	2134	2012	-10	-2	1	937	955	11	-1	1	1513	1460	7	-16	2	414	365
7	-6	1	255	164	4	-4	1	268	292	-9	-2	1	1595	1517	12	-1	1	2409	2339	-9	-15	2	223	251
8	-6	1	2230	2044	5	-4	1	907	857	-8	-2	1	660	647	13	-1	1	1198	1177	-7	-15	2	294	291
9	-6	1	1306	1208	6	-4	1	2091	1866	-7	-2	1	3547	3578	15	-1	1	398	377	-5	-15	2	1699	1762
10	-6	1	1473	1353	7	-4	1	727	674	-6	-2	1	380	361	-12	0	1	1799	1719	-4	-15	2	727	743
11	-6	1	504	465	8	-4	1	926	863	-5	-2	1	2315	2315	-10	0	1	822	830	-3	-15	2	1981	2029
13	-6	1	822	764	9	-4	1	2102	2012	-4	-2	1	1842	1858	-8	0	1	4161	4067	-2	-15	2	380	370
14	-6	1	663	626	10	-4	1	1103	1027	-3	-2	1	950	945	-6	0	1	4320	4284	-1	-15	2	508	517
-15	-5	1	499	531	11	-4	1	990	930	-2	-2	1	1679	1687	-4	0	1	621	605	1	-15	2	676	680
-11	-5	1	1633	1629	13	-4	1	1321	1285	-1	-2	1	1611	1765	-2	0	1	383	364	2	-15	2	230	202
-10	-5	1	669	690	14	-4	1	290	325	0	-2	1	1259	1186	0	0	1	913	1185	5	-15	2	247	194
-9	-5	1	3095	3229	15	-4	1	1064	1017	1	-2	1	2520	2541	2	0	1	1650	1726	7	-15	2	593	565
-8	-5	1	428	431	-16	-3	1	491	515	2	-2	1	2533	2447	4	0	1	3268	3201	8	-15	2	751	728
-7	-5	1	1593	1644	-15	-3	1	426	428	3	-2	1	384	333	6	0	1	4497	4358	-11	-14	2	1232	1272
-6	-5	1	879	857	-14	-3	1	487	512	4	-2	1	710	727	8	0	1	2429	2224	-10	-14	2	348	343
-5	-5	1	1350	1420	-13	-3	1	1160	1146	5	-2	1	3509	3296	12	0	1	860	893	-9	-14	2	1389	1457
-3	-5	1	293	310	-12	-3	1	607	570	6	-2	1	1343	1307	14	0	1	762	730	-8	-14	2	499	495
-2	-5	1	1053	1071	-10	-3	1	2061	2063	7	-2	1	3118	2906	-3	-18	2	310	316	-7	-14	2	259	345
-1	-5	1	739	686	-9	-3	1	1322	1315	8	-2	1	1992	1872	-2	-18	2	880	895	-6	-14	2	221	255
1	-5	1	2247	2067	-8	-3	1	2402	2421	9	-2	1	660	593	-1	-18	2	657	674	-5	-14	2	746	781
3	-5	1	3796	3545	-7	-3	1	455	457	10	-2	1	1678	1581	0	-18	2	687	654	-3	-14	2	282	276
5	-5	1	1242	1193	-5	-3	1	555	490	12	-2	1	601	624	1	-18	2	789	793	-2	-14	2	272	270
6	-5	1	249	217	-4	-3	1	884	903	13	-2	1	627	645	2	-18	2	553	537	-1	-14	2	545	540
7	-5	1	1636	1528	-3	-3	1	481	475	14	-2	1	996	970	3	-18	2	654	646	0	-14	2	238	257
9	-5	1	1925	1769	-2	-3	1	171	157	-15	-1	1	485	496	-7	-17	2	474	505	1	-14	2	1426	1411
10	-5	1	249	283	-1	-3	1	3396	3426	-14	-1	1	1277	1267	-6	-17	2	309	313	2	-14	2	735	788
11	-5	1	251	213	0	-3	1	1659	1613	-13	-1	1	1324	1320	-5	-17	2	347	365	3	-14	2	1887	1887
12	-5	1	375	358	1	-3	1	2139	2040	-12	-1	1	1354	1413	-4	-17	2	1516	1558	4	-14	2	437	485
13	-5	1	594	552	2	-3	1	2432	2295	-11	-1	1	964	953	-2	-17	2	1030	1027	6	-14	2	434	450
15	-5	1	1318	1282	3	-3	1	1305	1246	-10	-1	1	1027	1023	-1	-17	2	339	342	7	-14	2	1083	1058
-16	-4	1	743	718	4	-3	1	1842	1717	-8	-1	1	1230	1250	0	-17	2	337	279	-11	-13	2	798	824
-15	-4	1	1379	1378	5	-3	1	1095	1016	-7	-1	1	1248	1211	1	-17	2	362	419	-10	-13	2	223	207
-14	-4	1	833	808	6	-3	1	206	177	-6	-1	1	1289	1262	2	-17	2	547	516	-9	-13	2	331	389
-13	-4	1	222	248	7	-3	1	1280	1239	-5	-1	1	1835	1789	3	-17	2	537	517	-8	-13	2	469	471
-11	-4	1	1901	1914	8	-3	1	1582	1465	-4	-1	1	1291	1300	5	-17	2	856	846	-7	-13	2	656	688
-10	-4	1	741	750	9	-3	1	545	521	-3	-1	1	1535	1581	-9	-16	2	553	602	-6	-13	2	1160	1181
-9	-4	1	876	920	10	-3	1	1057	954	-2	-1	1	3247	3355	-8	-16	2	632	694	-5	-13	2	675	667
-8	-4	1	1021	1036	11	-3	1	1522	1446	-1	-1	1	2048	2189	-7	-16	2	309	339	-4	-13	2	1907	1931
-7	-4	1	176	197	12	-3	1	584	564	0	-1	1	4005	4185	-6	-16	2	347	348	-3	-13	2	950	978
-6	-4	1	1110	1133	13	-3	1	983	949	1	-1	1	3254	3207	-5	-16	2	541	563	-2	-13	2	1459	1492
-5	-4	1	916	931	14	-3	1	1065	1077	2	-1	1	454	381	-4	-16	2	301	321	-1	-13	2	551	526
-4	-4	1	1189	1239	15	-3	1	255	189	3	-1	1	1186	1056	-3	-16	2	258	235	1	-13	2	805	837
-3	-4	1	3036	3178	-16	-2	1	711	715	4	-1	1	478	482	-1	-16	2	772	779	3	-13	2	736	707
-2	-4	1	1866	1915	-14	-2	1	936	937	5	-1	1	274	275	0	-16	2	537	548	4	-13	2	485	382

H3DEP+ RE2(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC
5-13	2	1275	1206	12-11	2	563	558	12 -9	2	859	820	5 -7	2	2547	2485	5 -5	2	993	982
6-13	2	1060	1017	-14-10	2	1241	1327	-15 -8	2	585	568	6 -7	2	437	417	6 -5	2	244	276
7-13	2	438	453	-13-10	2	479	413	-14 -8	2	694	727	7 -7	2	302	308	7 -5	2	1875	1795
8-13	2	1245	1237	-12-10	2	801	867	-13 -8	2	1049	1134	8 -7	2	1910	1847	8 -5	2	345	330
9-13	2	834	764	-11-10	2	215	270	-11 -8	2	674	737	10 -7	2	1428	1371	9 -5	2	2349	2331
10-13	2	734	739	-8-10	2	574	613	-10 -8	2	1712	1826	12 -7	2	691	696	11 -5	2	329	273
-13-12	2	915	949	-7-10	2	477	434	-9 -8	2	665	630	13 -7	2	598	553	13 -5	2	1233	1216
-12-12	2	330	386	-6-10	2	1523	1633	-8 -8	2	876	921	-15 -6	2	541	503	-12 -4	2	813	836
-11-12	2	231	239	-5-10	2	846	876	-7 -8	2	1308	1338	-13 -6	2	227	214	-11 -4	2	1547	1629
-10-12	2	914	990	-4-10	2	210	217	-6 -8	2	1133	1195	-12 -6	2	888	927	-10 -4	2	1243	1316
-8-12	2	588	634	-3-10	2	749	748	-5 -8	2	273	283	-11 -6	2	1903	1906	-9 -4	2	2750	2839
-7-12	2	992	1071	-2-10	2	2746	2649	-4 -8	2	686	727	-10 -6	2	2093	2182	-8 -4	2	869	891
-6-12	2	239	306	-1-10	2	890	918	-3 -8	2	942	972	-9 -6	2	1858	1918	-5 -4	2	711	760
-5-12	2	1061	1124	0-10	2	2917	2850	-2 -8	2	2500	2619	-8 -6	2	1707	1799	-4 -4	2	829	790
-3-12	2	1270	1304	2-10	2	419	429	-1 -8	2	2496	2532	-7 -6	2	565	600	-3 -4	2	719	669
-1-12	2	2241	2271	3-10	2	402	393	0 -8	2	747	745	-5 -6	2	1346	1397	-2 -4	2	2029	2051
1-12	2	717	693	4-10	2	1163	1106	1 -8	2	2295	2212	-4 -6	2	1307	1372	-1 -4	2	331	326
2-12	2	1415	1417	5-10	2	292	267	2 -8	2	1627	1584	-3 -6	2	1568	1564	0 -4	2	772	786
3-12	2	253	232	6-10	2	1873	1809	3 -8	2	1477	1453	-1 -6	2	2687	2677	1 -4	2	3095	3021
4-12	2	505	479	7-10	2	346	308	4 -8	2	1986	1875	0 -6	2	2909	2888	2 -4	2	1937	1946
5-12	2	917	898	8-10	2	951	918	5 -8	2	1691	1620	1 -6	2	1170	1161	3 -4	2	3709	3602
6-12	2	782	740	9-10	2	273	216	6 -8	2	891	830	2 -6	2	2939	2843	4 -4	2	1139	1092
7-12	2	1277	1237	10-10	2	1475	1429	7 -8	2	1205	1189	3 -6	2	2586	2515	5 -4	2	196	121
8-12	2	318	346	11-10	2	363	370	8 -8	2	747	716	4 -6	2	1379	1323	6 -4	2	669	598
9-12	2	393	394	12-10	2	1418	1408	9 -8	2	494	473	5 -6	2	969	833	7 -4	2	1662	1593
11-12	2	1281	1265	-15 -9	2	247	247	10 -8	2	510	467	6 -6	2	341	314	8 -4	2	700	695
-13-11	2	770	845	-14 -9	2	306	477	11 -8	2	950	906	7 -6	2	1149	1100	9 -4	2	301	228
-12-11	2	731	772	-13 -9	2	356	361	12 -8	2	424	419	8 -6	2	502	500	10 -4	2	529	509
-11-11	2	662	639	-12 -9	2	1400	1492	13 -8	2	973	919	11 -6	2	643	621	11 -4	2	750	719
-10-11	2	235	205	-9 -9	2	216	206	-14 -7	2	683	740	12 -6	2	522	460	12 -4	2	486	464
-9-11	2	1053	1149	-8 -9	2	2339	2493	-13 -7	2	752	744	13 -6	2	422	433	13 -4	2	588	571
-8-11	2	896	963	-7 -9	2	707	751	-12 -7	2	414	425	14 -6	2	349	357	14 -4	2	454	380
-7-11	2	1611	1712	-6 -9	2	1073	1145	-11 -7	2	535	560	-15 -5	2	1639	1693	-16 -3	2	1357	1384
-6-11	2	829	875	-5 -9	2	546	575	-9 -7	2	1118	1160	-11 -5	2	958	999	-15 -3	2	400	365
-5-11	2	897	923	-4 -9	2	558	552	-8 -7	2	204	177	-10 -5	2	379	414	-14 -3	2	1055	1083
-4-11	2	294	312	-3 -9	2	1256	1290	-7 -7	2	1347	1426	-8 -5	2	237	233	-13 -3	2	898	901
-3-11	2	251	232	-2 -9	2	304	273	-6 -7	2	618	658	-7 -5	2	659	674	-12 -3	2	212	188
-2-11	2	182	135	-1 -9	2	137	93	-5 -7	2	161	175	-5 -5	2	2666	2776	-11 -3	2	763	766
-1-11	2	1163	1138	0 -9	2	2065	2025	-4 -7	2	3171	3277	-4 -5	2	177	158	-10 -3	2	273	340
0-11	2	704	639	2 -9	2	964	943	-3 -7	2	627	622	-3 -5	2	2854	2968	-9 -3	2	1700	1720
1-11	2	1108	1119	3 -9	2	1362	1282	-2 -7	2	2151	2183	-2 -5	2	695	713	-8 -3	2	265	234
3-11	2	745	727	4 -9	2	2395	2340	-1 -7	2	250	240	-1 -5	2	785	803	-7 -3	2	2162	2165
4-11	2	1372	1313	5 -9	2	828	784	0 -7	2	799	753	0 -5	2	1378	1351	-6 -3	2	2622	2618
5-11	2	2217	2224	6 -9	2	2514	2388	1 -7	2	2168	2085	1 -5	2	1860	1815	-5 -3	2	791	767
6-11	2	1240	1218	7 -9	2	1105	1097	2 -7	2	1020	994	2 -5	2	550	519	-4 -3	2	2251	2365
7-11	2	1537	1459	9 -9	2	680	635	3 -7	2	1344	1309	3 -5	2	577	549	-3 -3	2	4146	4319
11-11	2	589	584	11 -9	2	416	377	4 -7	2	215	174	4 -5	2	602	551	-2 -3	2	3709	3814

H3OEP+ RE2(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-1	-3	2	803	810	-12	-1	2	1788	1779	-1	-17	3	665	670	-9	-13	3	410	374	-1	-11	3	1498	1464
0	-3	2	573	525	-11	-1	2	700	718	0	-17	3	266	244	-8	-13	3	778	857	0	-11	3	753	743
1	-3	2	1939	1998	-9	-1	2	805	829	1	-17	3	232	231	-7	-13	3	588	607	1	-11	3	583	607
2	-3	2	1108	1074	-8	-1	2	3004	2965	2	-17	3	1325	1329	-6	-13	3	339	396	2	-11	3	219	245
3	-3	2	1276	1197	-7	-1	2	2220	2215	3	-17	3	406	409	-5	-13	3	339	361	3	-11	3	722	722
4	-3	2	336	354	-6	-1	2	2229	2211	4	-17	3	705	689	-4	-13	3	381	387	4	-11	3	770	740
5	-3	2	2216	2237	-5	-1	2	3124	3061	-9	-16	3	363	440	-3	-13	3	1333	1362	5	-11	3	1240	1204
6	-3	2	1225	1184	-3	-1	2	1621	1545	-6	-16	3	786	813	-1	-13	3	759	762	6	-11	3	1234	1197
7	-3	2	658	652	-2	-1	2	160	25	-5	-16	3	848	866	0	-13	3	737	745	7	-11	3	830	805
8	-3	2	2393	2328	-1	-1	2	1531	1515	-4	-16	3	1553	1607	1	-13	3	1093	1085	8	-11	3	253	254
9	-3	2	512	550	0	-1	2	3454	3587	-3	-16	3	765	806	2	-13	3	1496	1525	9	-11	3	553	575
10	-3	2	1040	998	1	-1	2	993	1046	-2	-16	3	650	672	3	-13	3	563	516	10	-11	3	1206	1164
11	-3	2	505	511	2	-1	2	816	841	0	-16	3	265	246	4	-13	3	1255	1270	11	-11	3	1022	1007
12	-3	2	492	460	3	-1	2	791	793	1	-16	3	638	610	5	-13	3	722	703	-14	-10	3	882	916
13	-3	2	1068	1015	4	-1	2	4289	4257	3	-16	3	381	392	7	-13	3	836	796	-13	-10	3	220	250
14	-3	2	702	688	5	-1	2	2108	2132	5	-16	3	555	601	9	-13	3	724	694	-12	-10	3	1341	1399
-15	-2	2	633	704	6	-1	2	2699	2600	6	-16	3	702	684	-13	-12	3	1014	1096	-9	-10	3	725	750
-14	-2	2	624	627	7	-1	2	1800	1840	-10	-15	3	354	358	-12	-12	3	270	291	-8	-10	3	1522	1588
-13	-2	2	1005	1013	9	-1	2	1196	1187	-9	-15	3	1075	1133	-11	-12	3	545	57[illegible]	-7	-10	3	513	528
-11	-2	2	428	446	11	-1	2	972	955	-3	-15	3	943	965	-9	-12	3	1010	103[illegible]	-6	-10	3	530	497
-10	-2	2	2679	2681	12	-1	2	909	928	-2	-15	3	386	383	-7	-12	3	914	986	-4	-10	3	248	205
-9	-2	2	324	305	13	-1	2	757	719	-1	-15	3	401	409	-6	-12	3	1018	1041	-3	-10	3	292	260
-8	-2	2	1531	1545	14	-1	2	859	862	0	-15	3	402	411	-4	-12	3	1314	1356	-2	-10	3	1613	1642
-7	-2	2	1698	1702	-14	0	2	1506	1478	1	-15	3	1387	1372	-3	-12	3	433	475	-1	-10	3	826	870
-6	-2	2	438	483	-12	0	2	601	638	2	-15	3	627	661	-2	-12	3	448	466	0	-10	3	2404	2426
-5	-2	2	728	702	-10	0	2	1129	1056	3	-15	3	1481	1475	-1	-12	3	1786	1759	1	-10	3	352	355
-4	-2	2	626	620	-8	0	2	1143	1092	4	-15	3	388	397	0	-12	3	188	136	2	-10	3	253	238
-3	-2	2	3369	3442	-6	0	2	3560	3479	7	-15	3	299	236	1	-12	3	1034	1024	3	-10	3	426	443
-2	-2	2	1798	1881	-4	0	2	1107	1018	-11	-14	3	279	270	2	-12	3	293	277	4	-10	3	2496	2404
-1	-2	2	4625	4901	-2	0	2	5024	4962	-9	-14	3	576	607	3	-12	3	1146	1102	5	-10	3	751	783
0	-2	2	601	582	0	0	2	4853	5127	-8	-14	3	382	392	4	-12	3	562	570	6	-10	3	1134	1075
1	-2	2	2034	2086	4	0	2	421	366	-7	-14	3	397	403	5	-12	3	1131	1064	7	-10	3	447	431
2	-2	2	2553	2469	6	0	2	2941	2921	-6	-14	3	505	552	6	-12	3	545	541	10	-10	3	679	658
3	-2	2	560	537	8	0	2	626	647	-5	-14	3	1929	1987	7	-12	3	230	216	-14	-9	3	699	917
4	-2	2	1917	1896	10	0	2	1973	1949	-4	-14	3	730	759	8	-12	3	1426	1418	-13	-9	3	613	661
5	-2	2	1406	1362	12	0	2	2019	1972	-3	-14	3	1776	1833	9	-12	3	289	279	-11	-9	3	741	784
6	-2	2	1102	1047	14	0	2	435	372	-2	-14	3	930	944	-14	-11	3	599	662	-10	-9	3	551	564
7	-2	2	1595	1560	-5	-18	3	818	799	-1	-14		238	240	-13	-11	3	494	467	-9	-9	3	424	440
8	-2	2	508	492	-4	-18	3	849	859	0	-14		525	514	-10	-11	3	547	526	-8	-9	3	1174	1219
10	-2	2	810	757	-3	-18	3	768	740	1	-14	3	209	126	-9	-11	3	590	615	-7	-9	3	394	461
11	-2	2	1754	1579	-1	-18	3	503	494	3	-14	3	631	639	-6	-11	3	413	406	-6	-9	3	2309	2410
13	-2	2	1257	1213	0	-18	3	964	970	6	-14	3	453	437	-7	-11	3	1731	1789	-4	-9	3	437	431
14	-2	2	1088	1121	-7	-17	3	521	509	7	-14	3	1384	1330	-6	-11	3	840	852	-3	-9	3	463	469
-16	-1	2	528	530	-6	-17	3	297	311	8	-14	3	322	268	-5	-11	3	1160	1200	-2	-9	3	2987	3070
-15	-1	2	565	553	-5	-17	3	231	288	-12	-13	3	633	649	-4	-11	3	599	616	-1	-9	3	816	856
-14	-1	2	591	552	-3	-17	3	421	414	-11	-13	3	460	481	-3	-11	3	1038	1030	0	-9	3	1303	1274
-13	-1	2	1271	1265	-2	-17	3	737	725	-10	-13	3	1099	1162	-2	-11	3	1607	1638	1	-9	3	1138	1103

H3OEP+ RE2(CO)6CL3-   MO DATA 0-40 DEG IN 2THETA   10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
2	-9	3	397	410	-3	-7	3	2336	2370	-9	-5	3	2240	2334	-12	-3	3	1349	1336	5	-2	3	3131	3023
3	-9	3	656	685	-2	-7	3	344	343	-8	-5	3	187	148	-11	-3	3	834	836	6	-2	3	382	363
4	-9	3	660	647	-1	-7	3	2223	2274	-7	-5	3	477	441	-10	-3	3	2416	2447	7	-2	3	2013	1966
5	-9	3	1069	1075	0	-7	3	2611	2513	-5	-5	3	294	292	-9	-3	3	479	489	8	-2	3	1631	1545
6	-9	3	1774	1769	1	-7	3	581	558	-4	-5	3	1064	1097	-8	-3	3	1956	1995	9	-2	3	804	767
8	-9	3	390	363	2	-7	3	3219	3171	-3	-5	3	1512	1561	-7	-3	3	1490	1521	11	-2	3	1583	1615
9	-9	3	451	411	3	-7	3	663	609	-2	-5	3	888	844	-6	-3	3	640	645	12	-2	3	908	912
10	-9	3	1557	1512	4	-7	3	1115	1124	-1	-5	3	904	906	-5	-3	3	735	787	13	-2	3	523	564
11	-9	3	885	843	5	-7	3	1196	1195	0	-5	3	785	762	-4	-3	3	2306	2225	14	-2	3	269	264
12	-9	3	868	821	6	-7	3	657	716	1	-5	3	2995	3016	-3	-3	3	210	197	-16	-1	3	444	460
-15	-8	3	655	679	7	-7	3	863	841	2	-5	3	1008	1029	-2	-3	3	187	144	-15	-1	3	278	280
-14	-8	3	551	572	9	-7	3	722	726	3	-5	3	3467	3485	-1	-3	3	1904	1925	-14	-1	3	1131	1107
-13	-8	3	889	923	10	-7	3	385	376	4	-5	3	397	397	0	-3	3	2008	2020	-13	-1	3	662	636
-12	-8	3	774	803	11	-7	3	972	954	5	-5	3	272	279	1	-3	3	161	164	-12	-1	3	535	519
-11	-8	3	555	563	12	-7	3	695	701	7	-5	3	1038	982	2	-3	3	3430	3429	-11	-1	3	223	244
-10	-8	3	934	969	13	-7	3	368	432	8	-5	3	281	250	3	-3	3	1533	1499	-10	-1	3	852	834
-9	-8	3	661	693	-16	-6	3	1045	1051	9	-5	3	755	778	4	-3	3	1154	1178	-9	-1	3	1199	1209
-8	-8	3	1654	1727	-15	-6	3	616	586	12	-5	3	326	253	5	-3	3	1210	1198	-8	-1	3	1362	1259
-7	-8	3	1152	1166	-14	-6	3	507	518	13	-5	3	1516	1543	6	-3	3	213	159	-7	-1	3	1977	1963
-6	-8	3	903	964	-13	-6	3	512	528	-16	-4	3	522	530	7	-3	3	1339	1312	-6	-1	3	3121	3065
-4	-8	3	2322	2434	-11	-6	3	367	341	-15	-4	3	761	778	8	-3	3	382	367	-5	-1	3	726	689
-3	-8	3	1255	1305	-10	-6	3	596	557	-14	-4	3	633	646	9	-3	3	651	647	-4	-1	3	648	626
-2	-8	3	186	146	-9	-6	3	1124	1169	-13	-4	3	381	366	10	-3	3	359	317	-3	-1	3	1271	1262
-1	-8	3	1874	1943	-8	-6	3	198	201	-12	-4	3	512	528	11	-3	3	854	827	-2	-1	3	2613	2653
0	-8	3	1024	1021	-7	-6	3	563	541	-9	-4	3	932	950	12	-3	3	710	667	-1	-1	3	587	584
1	-8	3	1378	1364	-6	-6	3	1155	1201	-8	-4	3	354	376	14	-3	3	1040	1062	0	-1	3	1270	1300
2	-8	3	416	410	-5	-6	3	2651	2867	-7	-4	3	203	181	-16	-2	3	908	997	1	-1	3	1848	1879
3	-8	3	665	648	-4	-6	3	2860	2987	-6	-4	3	1533	1523	-15	-2	3	602	608	2	-1	3	2079	2056
4	-8	3	1559	1548	-3	-6	3	2691	2685	-5	-4	3	3015	3116	-14	-2	3	283	262	3	-1	3	581	539
5	-8	3	1665	1634	-2	-6	3	1903	1942	-4	-4	3	3441	3566	-13	-2	3	1737	1753	4	-1	3	762	766
6	-8	3	506	499	-1	-6	3	536	533	-3	-4	3	995	1084	-12	-2	3	762	758	5	-1	3	1628	1656
7	-8	3	1059	1062	1	-6	3	932	904	-2	-4	3	2614	2654	-11	-2	3	214	268	6	-1	3	2780	2803
8	-8	3	1131	1096	2	-6	3	520	511	0	-4	3	1139	1151	-10	-2	3	467	445	7	-1	3	1149	1205
9	-8	3	1018	989	3	-6	3	1026	1016	1	-4	3	586	564	-9	-2	3	1315	1303	8	-1	3	430	400
11	-8	3	960	935	4	-6	3	663	621	2	-4	3	320	288	-8	-2	3	1325	1314	9	-1	3	272	277
12	-8	3	572	548	5	-6	3	887	850	3	-4	3	2159	2059	-7	-2	3	2079	2062	10	-1	3	1572	1587
-15	-7	3	712	730	6	-6	3	970	997	4	-4	3	416	402	-6	-2	3	988	959	11	-1	3	778	744
-14	-7	3	224	245	7	-6	3	1209	1175	5	-4	3	349	395	-5	-2	3	1351	1318	12	-1	3	460	403
-13	-7	3	329	279	8	-6	3	1871	1827	6	-4	3	1463	1393	-4	-2	3	2582	2629	13	-1	3	770	732
-12	-7	3	1304	1348	9	-6	3	1292	1289	7	-4	3	1867	1824	-3	-2	3	697	742	-16	0	3	228	231
-11	-7	3	534	566	10	-6	3	942	929	8	-4	3	1602	1607	-2	-2	3	503	535	-14	0	3	1535	1524
-10	-7	3	2193	2309	13	-6	3	690	697	9	-4	3	2056	2029	-1	-2	3	2530	2626	-12	0	3	1918	1935
-8	-7	3	754	806	-15	-5	3	265	286	10	-4	3	1141	1124	0	-2	3	1012	1003	-10	0	3	1196	1157
-7	-7	3	1817	1858	-13	-5	3	663	712	11	-4	3	251	286	1	-2	3	715	707	-8	0	3	3295	3246
-6	-7	3	342	340	-12	-5	3	243	273	13	-4	3	585	579	2	-2	3	1529	1487	-6	0	3	753	745
-5	-7	3	1124	1204	-11	-5	3	2728	2784	-17	-3	3	416	378	3	-2	3	2069	2071	-5	0	3	159	0
-4	-7	3	482	526	-10	-5	3	618	641	-15	-3	3	898	903	4	-2	3	1958	1917	-4	0	3	1084	1827

H3OEP+ RE2(CO)6CL3-   MO DATA   0-40 DEG IN 2THETA   10 FO AND 10FC   PAGE 7

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-2	0	3	4086	4081	-1	-14	4	304	285	-8	-11	4	239	259	-5	-9	4	1174	1213	-10	-7	4	1061	1141
0	0	3	4542	4714	0	-14	4	344	324	-7	-11	4	756	762	-4	-9	4	427	443	-9	-7	4	1073	1128
2	0	3	220	192	1	-14	4	1877	1824	-6	-11	4	525	553	-3	-9	4	1180	1191	-6	-7	4	1471	1545
4	0	3	4409	4455	2	-14	4	527	486	-5	-11	4	242	213	-2	-9	4	1493	1557	-5	-7	4	314	297
6	0	3	2607	2632	3	-14	4	1209	1220	-4	-11	4	246	291	-1	-9	4	1469	1460	-4	-7	4	2528	2658
8	0	3	949	917	4	-14	4	564	565	-3	-11	4	1174	1212	0	-9	4	1948	1981	-3	-7	4	318	353
10	0	3	1281	1259	6	-14	4	518	517	-2	-11	4	1502	1509	1	-9	4	749	748	-2	-7	4	660	687
12	0	3	1209	1234	7	-14	4	323	269	-1	-11	4	1851	1839	2	-9	4	495	482	-1	-7	4	1834	1844
-4	-18	4	597	602	-12	-13	4	339	372	0	-11	4	1226	1240	4	-9	4	1979	1962	1	-7	4	579	613
-2	-18	4	642	614	-10	-13	4	505	502	1	-11	4	798	793	5	-9	4	479	470	2	-7	4	1672	1692
-1	-18	4	528	563	-9	-13	4	595	642	2	-11	4	819	816	6	-9	4	262	236	3	-7	4	1415	1360
-6	-17	4	879	925	-7	-13	4	342	334	3	-11	4	1297	1298	7	-9	4	740	759	4	-7	4	655	644
-4	-17	4	1217	1209	-6	-13	4	868	865	4	-11	4	1371	1341	9	-9	4	870	881	5	-7	4	1195	1171
-1	-17	4	461	438	-5	-13	4	1085	1107	5	-11	4	1009	995	10	-9	4	1024	1030	6	-7	4	1376	1364
0	-17	4	277	250	-4	-13	4	1198	1218	6	-11	4	377	331	11	-9	4	543	543	8	-7	4	1842	1824
2	-17	4	318	326	-2	-13	4	1193	1177	7	-11	4	259	317	-15	-8	4	419	494	9	-7	4	455	429
3	-17	4	370	344	-1	-13	4	1365	1350	9	-11	4	475	479	-14	-8	4	293	311	10	-7	4	568	582
-9	-16	4	278	253	0	-13	4	396	401	10	-11	4	826	787	-12	-8	4	1200	1307	11	-7	4	846	853
-8	-16	4	232	241	2	-13	4	538	517	-14	-10	4	581	582	-11	-8	4	303	264	-16	-6	4	391	363
-7	-16	4	427	389	3	-13	4	1028	998	-12	-10	4	438	488	-10	-8	4	973	1006	-15	-6	4	718	742
-5	-16	4	315	294	6	-13	4	694	641	-11	-10	4	397	391	-9	-8	4	882	921	-13	-6	4	726	746
-4	-16	4	754	747	7	-13	4	836	822	-10	-10	4	373	398	-8	-8	4	1000	1054	-12	-6	4	1111	1153
-3	-16	4	841	842	8	-13	4	765	754	-9	-10	4	334	348	-7	-8	4	1288	1331	-11	-6	4	2032	2095
-2	-16	4	342	337	-12	-12	4	834	867	-8	-10	4	1701	1776	-6	-8	4	872	864	-10	-6	4	1218	1235
0	-16	4	1055	1053	-11	-12	4	239	183	-7	-10	4	889	932	-5	-8	4	235	243	-9	-6	4	667	685
1	-16	4	705	705	-10	-12	4	1178	1189	-6	-10	4	1060	1127	-4	-8	4	1315	1346	-8	-6	4	501	525
2	-16	4	1298	1290	-9	-12	4	815	867	-5	-10	4	420	414	-3	-8	4	985	993	-7	-6	4	394	438
3	-16	4	436	409	-8	-12	4	202	187	-4	-10	4	691	693	-2	-8	4	1332	1339	-5	-6	4	560	572
4	-16	4	450	460	-7	-12	4	1698	1735	-3	-10	4	779	785	-1	-8	4	1238	1241	-4	-6	4	969	961
-9	-15	4	821	866	-6	-12	4	601	627	-2	-10	4	1087	1866	0	-8	4	1200	1204	-3	-6	4	1976	2040
-7	-15	4	689	717	-5	-12	4	353	369	-1	-10	4	687	690	1	-8	4	1193	1172	-2	-6	4	1066	1053
-6	-15	4	347	380	-4	-12	4	832	868	1	-10	4	280	275	2	-8	4	2052	2029	0	-6	4	1871	1879
-5	-15	4	1654	1725	-3	-12	4	1079	1073	2	-10	4	233	235	3	-8	4	862	865	1	-6	4	2893	2898
-4	-15	4	401	436	-2	-12	4	325	333	4	-10	4	2133	2108	4	-8	4	389	354	2	-6	4	1922	1923
-3	-15	4	1104	1106	-1	-12	4	366	338	5	-10	4	431	417	5	-8	4	1553	1564	3	-6	4	1322	1329
-1	-15	4	315	312	0	-12	4	1045	1027	6	-10	4	1647	1625	6	-8	4	1143	1152	4	-6	4	287	315
0	-15	4	215	208	2	-12	4	1212	1202	7	-10	4	455	466	7	-8	4	306	345	5	-6	4	645	602
1	-15	4	249	247	3	-12	4	1031	1036	8	-10	4	325	310	8	-8	4	494	481	6	-6	4	424	392
3	-15	4	859	843	4	-12	4	528	568	10	-10	4	956	941	9	-8	4	460	448	8	-6	4	763	764
6	-15	4	252	276	5	-12	4	1954	1941	-15	-9	4	443	443	10	-8	4	868	836	9	-6	4	944	965
-11	-14	4	1260	1349	7	-12	4	573	579	-14	-9	4	1567	1625	11	-8	4	507	467	11	-6	4	303	315
-10	-14	4	499	478	8	-12	4	615	626	-13	-9	4	708	719	-16	-7	4	847	882	12	-6	4	505	550
-9	-14	4	710	731	9	-12	4	645	658	-12	-9	4	899	925	-15	-7	4	856	914	-16	-5	4	275	278
-8	-14	4	309	339	-14	-11	4	845	883	-11	-9	4	482	497	-14	-7	4	323	282	-15	-5	4	785	802
-6	-14	4	390	420	-13	-11	4	1115	1169	-10	-9	4	921	982	-13	-7	4	1192	1227	-13	-5	4	246	162
-5	-14	4	741	765	-12	-11	4	815	851	-8	-9	4	1307	1364	-12	-7	4	289	295	-12	-5	4	345	352
-3	-14	4	970	1017	-9	-11	4	663	681	-6	-9	4	663	671	-11	-7	4	191	160	-11	-5	4	700	672

H3DEP+ RE2(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC PAGE 8

H	K	L	FOBS	FCALC
-10	-5	4	264	308
-9	-5	4	1306	1349
-7	-5	4	1177	1183
-6	-5	4	926	922
-5	-5	4	3530	3613
-4	-5	4	1507	1495
-3	-5	4	2213	2300
-2	-5	4	585	577
-1	-5	4	1014	990
0	-5	4	198	169
1	-5	4	1007	991
2	-5	4	865	862
3	-5	4	2342	2398
4	-5	4	223	216
6	-5	4	256	270
7	-5	4	2642	2840
8	-5	4	528	548
9	-5	4	1253	1268
-16	-4	4	401	398
-15	-4	4	792	790
-13	-4	4	687	693
-12	-4	4	1233	1232
-11	-4	4	2091	2084
-10	-4	4	1582	1603
-9	-4	4	826	864
-8	-4	4	891	916
-7	-4	4	706	675
-6	-4	4	1199	1203
-5	-4	4	182	89
-4	-4	4	352	392
-3	-4	4	1916	1985
-1	-4	4	672	657
0	-4	4	2631	2600
1	-4	4	2812	2983
2	-4	4	2436	2440
3	-4	4	1788	1803
4	-4	4	1117	1138
5	-4	4	1638	1584
6	-4	4	728	740
8	-4	4	556	579
9	-4	4	1294	1288
10	-4	4	243	275
12	-4	4	505	488
13	-4	4	1308	1360
-17	-3	4	543	541
-16	-3	4	1121	1112
-15	-3	4	220	187

H	K	L	FOBS	FCALC
-14	-3	4	322	337
-13	-3	4	1058	1011
-12	-3	4	605	605
-10	-3	4	648	681
-9	-3	4	1091	1071
-8	-3	4	361	357
-7	-3	4	810	799
-6	-3	4	2613	2677
-5	-3	4	2427	2442
-4	-3	4	2559	2634
-2	-3	4	1450	1461
-1	-3	4	1667	1705
0	-3	4	1686	1684
1	-3	4	172	154
2	-3	4	1109	1134
3	-3	4	2531	2593
4	-3	4	1124	1086
5	-3	4	1215	1232
6	-3	4	1738	1783
7	-3	4	732	810
8	-3	4	2114	2161
9	-3	4	242	243
10	-3	4	554	568
11	-3	4	971	996
13	-3	4	495	500
-16	-2	4	425	447
-15	-2	4	372	308
-14	-2	4	446	424
-13	-2	4	361	350
-12	-2	4	1103	1125
-10	-2	4	1132	1100
-9	-2	4	1999	1981
-8	-2	4	267	315
-7	-2	4	3576	3557
-6	-2	4	607	769
-5	-2	4	895	906
-4	-2	4	1867	1858
-3	-2	4	1682	1661
-2	-2	4	145	160
-1	-2	4	2053	2035
0	-2	4	1078	1135
1	-2	4	631	614
2	-2	4	1362	1413
3	-2	4	1331	1362
4	-2	4	666	654
5	-2	4	2400	2387
6	-2	4	813	859

H	K	L	FOBS	FCALC
7	-2	4	1173	1156
8	-2	4	1051	1087
9	-2	4	362	402
10	-2	4	1005	997
11	-2	4	941	943
12	-2	4	236	164
13	-2	4	484	460
-17	-1	4	238	213
-15	-1	4	837	831
-14	-1	4	1362	1346
-13	-1	4	1429	1395
-12	-1	4	1309	1330
-11	-1	4	352	309
-10	-1	4	1687	1627
-9	-1	4	1066	1065
-8	-1	4	1460	1446
-7	-1	4	842	826
-6	-1	4	1673	1629
-5	-1	4	532	523
-4	-1	4	1641	1608
-3	-1	4	550	526
-2	-1	4	2212	2246
-1	-1	4	2356	2434
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2	-1	4	1137	1145
3	-1	4	198	214
4	-1	4	2218	2297
5	-1	4	1238	1229
6	-1	4	214	237
7	-1	4	233	286
8	-1	4	211	183
9	-1	4	948	948
10	-1	4	1104	1137
11	-1	4	1162	1212
12	-1	4	1279	1287
13	-1	4	351	355
-16	0	4	739	733
-14	0	4	413	382
-12	0	4	824	817
-10	0	4	535	556
-8	0	4	3737	3657
-6	0	4	3187	3089
-4	0	4	2338	2255
-2	0	4	2660	2664
0	0	4	891	878
2	0	4	813	802

H	K	L	FOBS	FCALC
4	0	4	2739	2725
6	0	4	2844	2919
8	0	4	390	354
10	0	4	838	826
12	0	4	272	325
-6	-17	5	262	284
-5	-17	5	230	204
-4	-17	5	802	810
-3	-17	5	230	170
-2	-17	5	289	283
0	-17	5	899	864
-7	-16	5	423	412
-6	-16	5	937	961
-5	-16	5	738	742
-4	-16	5	1035	1066
-1	-16	5	397	377
1	-16	5	314	300
2	-16	5	735	743
3	-16	5	778	748
-10	-15	5	289	252
-8	-15	5	220	119
-5	-15	5	927	957
-4	-15	5	242	273
-3	-15	5	952	966
-1	-15	5	656	646
0	-15	5	655	643
1	-15	5	1519	1522
2	-15	5	312	355
3	-15	5	837	863
4	-15	5	335	314
-11	-14	5	761	758
-9	-14	5	723	747
-7	-14	5	701	719
-6	-14	5	233	254
-5	-14	5	1297	1300
-4	-14	5	664	687
-3	-14	5	408	380
-2	-14	5	530	550
0	-14	5	542	552
1	-14	5	1196	1209
2	-14	5	255	295
3	-14	5	995	1000
5	-14	5	820	795
-12	-13	5	701	731
-11	-13	5	445	436
-10	-13	5	883	925
-9	-13	5	533	554

H	K	L	FOBS	FCALC
-8	-13	5	741	773
-7	-13	5	563	553
-6	-13	5	772	796
-5	-13	5	773	805
-4	-13	5	898	893
-3	-13	5	717	691
-1	-13	5	782	748
0	-13	5	762	764
1	-13	5	1194	1204
2	-13	5	1128	1134
3	-13	5	427	429
4	-13	5	651	637
5	-13	5	936	923
6	-13	5	759	763
-13	-12	5	891	887
-12	-12	5	318	295
-10	-12	5	416	441
-9	-12	5	531	517
-7	-12	5	362	400
-6	-12	5	1092	1078
-4	-12	5	848	869
-3	-12	5	1550	1601
-1	-12	5	1677	1697
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2	-12	5	1086	1102
3	-12	5	647	633
4	-12	5	283	242
6	-12	5	627	565
7	-12	5	243	280
8	-12	5	587	602
-12	-11	5	860	894
-9	-11	5	1417	1514
-8	-11	5	979	1031
-7	-11	5	1414	1474
-6	-11	5	547	569
-5	-11	5	206	235
-4	-11	5	532	502
-3	-11	5	458	472
-2	-11	5	390	406
0	-11	5	963	968
1	-11	5	270	246
2	-11	5	195	167
3	-11	5	1200	1287
4	-11	5	1066	1012
5	-11	5	1385	1395
6	-11	5	532	536
8	-11	5	813	801

H3OEP+ RE2(CO)6CL3-   MO DATA   0-40 DEG IN 2THETA   10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-14	-10	5	1192	1257	-5	-8	5	593	615	-7	-6	5	2147	2219	-4	-4	5	1703	1777	-10	-2	5	1107	1076
-12	-10	5	751	799	-4	-8	5	511	513	-6	-6	5	1445	1496	-3	-4	5	159	124	-9	-2	5	536	497
-10	-10	5	589	616	-3	-8	5	2068	2122	-5	-6	5	2393	2482	-2	-4	5	1154	1161	-8	-2	5	851	840
-8	-10	5	259	223	-2	-8	5	735	756	-4	-6	5	1910	1922	0	-4	5	1661	1661	-7	-2	5	519	532
-7	-10	5	427	429	-1	-8	5	1761	1788	-2	-6	5	1271	1305	1	-4	5	2371	2350	-6	-2	5	2268	2253
-6	-10	5	705	722	1	-8	5	379	367	0	-6	5	2015	2063	2	-4	5	1087	1108	-5	-2	5	225	199
-4	-10	5	833	840	2	-8	5	1200	1209	1	-6	5	860	897	3	-4	5	1911	1978	-4	-2	5	338	356
-3	-10	5	634	618	3	-8	5	284	308	2	-6	5	1480	1507	4	-4	5	312	371	-3	-2	5	1271	1350
-2	-10	5	2779	2831	4	-8	5	738	716	3	-6	5	1595	1660	5	-4	5	604	637	-1	-2	5	2601	2701
-1	-10	5	844	858	5	-8	5	555	563	4	-6	5	362	339	6	-4	5	857	876	0	-2	5	635	636
0	-10	5	1306	1270	6	-8	5	659	656	6	-6	5	1645	1640	7	-4	5	2169	2216	1	-2	5	939	978
2	-10	5	620	593	7	-8	5	784	755	7	-6	5	1289	1298	8	-4	5	1098	1110	2	-2	5	1512	1500
3	-10	5	211	198	8	-8	5	707	713	8	-6	5	1421	1451	9	-4	5	324	303	3	-2	5	675	693
4	-10	5	1049	1052	9	-8	5	1162	1232	9	-6	5	405	368	10	-4	5	492	469	4	-2	5	536	569
5	-10	5	265	218	10	-8	5	549	578	10	-6	5	756	741	11	-4	5	317	331	5	-2	5	445	488
8	-10	5	308	524	-16	-7	5	710	714	-16	-5	5	338	344	12	-4	5	294	258	6	-2	5	1701	1633
-15	-9	5	317	312	-15	-7	5	240	247	-15	-5	5	636	646	-17	-3	5	336	384	8	-2	5	860	923
-12	-9	5	799	847	-13	-7	5	565	598	-13	-5	5	1098	1096	-16	-3	5	546	569	9	-2	5	1149	1158
-11	-9	5	332	314	-12	-7	5	1035	1073	-11	-5	5	1768	1776	-15	-3	5	501	506	10	-2	5	552	590
-10	-9	5	541	588	-11	-7	5	555	539	-9	-5	5	1087	1080	-13	-3	5	792	810	11	-2	5	1057	1082
-9	-9	5	661	671	-10	-7	5	958	1000	-7	-5	5	941	956	-12	-3	5	1285	1284	-16	-1	5	824	832
-8	-9	5	2170	2256	-9	-7	5	1053	1067	-5	-5	5	2077	2156	-11	-3	5	478	502	-14	-1	5	377	374
-7	-9	5	525	504	-7	-7	5	2197	2312	-4	-5	5	371	413	-10	-3	5	1513	1482	-12	-1	5	1037	1021
-6	-9	5	1469	1497	-6	-7	5	1863	1993	-3	-5	5	1775	1842	-9	-3	5	1231	1194	-11	-1	5	726	695
-5	-9	5	303	316	-5	-7	5	376	409	-1	-5	5	1873	1867	-8	-3	5	1233	1152	-10	-1	5	956	938
-4	-9	5	1157	1166	-4	-7	5	2197	2272	0	-5	5	678	656	-7	-3	5	2028	2033	-9	-1	5	1727	1671
-3	-9	5	280	271	-3	-7	5	941	970	1	-5	5	2327	2457	-6	-3	5	1474	1464	-8	-1	5	2907	2873
-2	-9	5	1106	1070	-2	-7	5	372	412	2	-5	5	306	293	-5	-3	5	834	843	-7	-1	5	2170	2132
-1	-9	5	186	229	0	-7	5	1929	1974	3	-5	5	915	926	-4	-3	5	2492	2558	-6	-1	5	1300	1309
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2	-9	5	359	369	3	-7	5	676	680	7	-5	5	1416	1443	1	-3	5	1363	1442	-3	-1	5	910	936
3	-9	5	453	423	4	-7	5	227	260	8	-5	5	439	487	2	-3	5	1921	1964	-2	-1	5	393	430
4	-9	5	1774	1761	5	-7	5	1266	1236	9	-5	5	1625	1661	3	-3	5	1032	1032	-1	-1	5	711	716
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6	-9	5	1049	1035	7	-7	5	358	367	-17	-4	5	793	815	5	-3	5	1849	1972	1	-1	5	1011	986
7	-9	5	341	359	8	-7	5	923	909	-16	-4	5	346	304	6	-3	5	952	948	2	-1	5	697	687
8	-9	5	613	605	9	-7	5	738	717	-14	-4	5	293	275	7	-3	5	221	85	3	-1	5	1685	1723
10	-9	5	775	771	-16	-6	5	356	370	-13	-4	5	206	194	8	-3	5	1231	1208	4	-1	5	2243	2365
-15	-8	5	958	979	-15	-6	5	346	339	-12	-4	5	939	914	9	-3	5	906	923	5	-1	5	1453	1540
-14	-8	5	896	969	-14	-6	5	403	414	-11	-4	5	1092	1099	10	-3	5	269	208	6	-1	5	1552	1589
-13	-8	5	1236	1265	-13	-6	5	220	236	-10	-4	5	652	673	12	-3	5	846	876	7	-1	5	590	601
-11	-8	5	209	205	-12	-6	5	836	837	-9	-4	5	648	631	-16	-2	5	300	300	8	-1	5	1029	1042
-10	-8	5	1289	1294	-11	-6	5	1042	1046	-8	-4	5	459	463	-15	-2	5	1410	1449	10	-1	5	695	719
-8	-8	5	368	373	-10	-6	5	801	831	-7	-4	5	1686	1726	-14	-2	5	691	668	11	-1	5	453	441
-7	-8	5	1028	1000	-9	-6	5	803	796	-6	-4	5	829	842	-13	-2	5	1484	1439	-16	0	5	774	815
-6	-8	5	2255	2357	-8	-6	5	460	447	-5	-4	5	2715	2790	-12	-2	5	262	317	-14	0	5	2396	2346

H3OEP+ RE2(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-12	0	5	746	701	-4	-13	6	562	573	-5	-10	6	608	618	5	-8	6	1428	1392	10	-6	6	335	368
-10	0	5	829	754	-3	-13	6	988	967	-4	-10	6	280	275	6	-8	6	486	473	-13	-5	6	406	415
-8	0	5	204	152	-2	-13	6	894	924	-3	-10	6	513	514	7	-8	6	565	563	-11	-5	6	1610	1622
-6	0	5	1865	1770	0	-13	6	1183	1200	-2	-10	6	516	513	8	-8	6	898	905	-9	-5	6	644	635
-4	0	5	202	155	1	-13	6	1188	1246	0	-10	6	888	920	9	-8	6	259	255	-8	-5	6	392	417
-2	0	5	2639	2656	2	-13	6	816	824	2	-10	6	1138	1148	-15	-7	6	1036	1061	-7	-5	6	2249	2305
0	0	5	2109	2082	3	-13	6	676	678	3	-10	6	543	598	-13	-7	6	376	417	-5	-5	6	1531	1576
2	0	5	1632	1628	4	-13	6	437	452	4	-10	6	2012	2002	-12	-7	6	1105	1146	-4	-5	6	355	348
4	0	5	904	900	5	-13	6	539	544	6	-10	6	890	891	-11	-7	6	712	779	-1	-5	6	813	863
8	0	5	794	816	6	-13	6	277	261	8	-10	6	302	264	-10	-7	6	1063	1077	1	-5	6	2751	2845
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12	0	5	859	931	-12	-12	6	707	769	-14	-9	6	1263	1343	-7	-7	6	428	420	3	-5	6	1647	1678
-6	-16	6	519	549	-9	-12	6	1098	1146	-13	-9	6	614	607	-6	-7	6	1876	1959	4	-5	6	237	96
-5	-16	6	486	481	-7	-12	6	883	918	-11	-9	6	416	425	-5	-7	6	731	765	5	-5	6	1402	1407
-4	-16	6	755	726	-6	-12	6	653	664	-10	-9	6	766	761	-4	-7	6	827	846	6	-5	6	539	560
-3	-16	6	464	481	-4	-12	6	672	696	-9	-9	6	452	481	-3	-7	6	1236	1266	7	-5	6	1636	1686
-1	-16	6	516	524	-2	-12	6	674	694	-8	-9	6	742	777	-2	-7	6	501	488	8	-5	6	665	674
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1	-16	6	518	489	0	-12	6	985	988	-5	-9	6	444	426	0	-7	6	1093	1118	-13	-4	6	980	988
-9	-15	6	568	594	2	-12	6	479	457	-4	-9	6	1161	1212	2	-7	6	1652	1646	-12	-4	6	439	462
-7	-15	6	838	857	3	-12	6	1404	1424	-3	-9	6	863	896	3	-7	6	560	572	-11	-4	6	806	764
-6	-15	6	367	363	5	-12	6	1039	1016	-2	-9	6	1951	2043	6	-7	6	1444	1436	-10	-4	6	508	516
-5	-15	6	856	858	6	-12	6	678	668	-1	-9	6	568	551	7	-7	6	347	379	-9	-4	6	259	268
-4	-15	6	239	272	-13	-11	6	628	645	0	-9	6	508	539	8	-7	6	433	384	-8	-4	6	823	847
-3	-15	6	318	305	-11	-11	6	270	255	2	-9	6	920	925	9	-7	6	663	641	-7	-4	6	867	885
-1	-15	6	487	492	-10	-11	6	333	341	5	-9	6	427	405	-16	-6	6	526	559	-6	-4	6	1128	1129
0	-15	6	312	306	-8	-11	6	644	686	6	-9	6	444	402	-13	-6	6	1047	1048	-5	-4	6	2259	2357
1	-15	6	1066	1049	-7	-11	6	845	884	8	-9	6	629	663	-12	-6	6	522	494	-4	-4	6	1016	1029
2	-15	6	630	627	-6	-11	6	487	520	9	-9	6	824	806	-11	-6	6	624	591	-3	-4	6	1434	1453
3	-15	6	760	740	-5	-11	6	182	217	-14	-8	6	605	630	-10	-6	6	800	805	-2	-4	6	153	152
-11	-14	6	508	471	-4	-11	6	531	544	-13	-8	6	216	177	-9	-6	6	684	687	-1	-4	6	1487	1566
-10	-14	6	299	351	-3	-11	6	1530	1599	-12	-8	6	894	899	-8	-6	6	304	313	0	-4	6	1443	1444
-8	-14	6	371	369	-2	-11	6	1052	1064	-11	-8	6	270	236	-6	-6	6	2028	2107	1	-4	6	1153	1207
-7	-14	6	257	303	-1	-11	6	1734	1719	-10	-8	6	446	435	-5	-6	6	1574	1613	2	-4	6	893	919
-6	-14	6	229	249	0	-11	6	240	234	-9	-8	6	1764	1797	-4	-6	6	1238	1290	4	-4	6	888	886
-5	-14	6	1293	1351	1	-11	6	366	408	-8	-8	6	750	792	-3	-6	6	975	976	6	-4	6	931	947
-1	-14	6	1106	1149	2	-11	6	1033	1050	-7	-8	6	1145	1158	-2	-6	6	155	106	7	-4	6	1794	1850
1	-14	6	962	944	6	-11	6	831	831	-6	-8	6	844	872	-1	-6	6	1246	1232	8	-4	6	719	727
2	-14	6	507	517	8	-11	6	333	270	-5	-8	6	721	772	0	-6	6	1225	1215	9	-4	6	1496	1646
4	-14	6	611	[illegible]	-14	-10	6	596	614	-4	-8	6	1591	1642	1	-6	6	1832	1799	11	-4	6	362	379
-12	-13	6	656	[illegible]	-12	-10	6	495	514	-3	-8	6	384	391	2	-6	6	585	617	-16	-3	6	403	331
-11	-13	6	604	[illegible]	-11	-10	6	218	179	-1	-8	6	348	344	3	-6	6	192	112	-15	-3	6	1073	1078
-10	-13	6	694	[illegible]	-10	-10	6	1146	1179	0	-8	6	1608	1642	4	-6	6	438	476	-14	-3	6	479	[illegible]
-8	-13	6	203	[illegible]	-9	-10	6	603	617	1	-8	6	558	557	6	-6	6	1158	1167	-13	-3	6	760	[illegible]
-7	-13	6	801	[illegible]	-8	-10	6	1925	2035	2	-8	6	577	577	7	-6	6	1417	1399	-12	-3	6	1160	[illegible]
-6	-13	6	583	[illegible]	-7	-10	6	565	598	3	-8	6	1516	1542	8	-6	6	1281	1289	-11	-3	6	517	[illegible]
-5	-13	6	292	326	-6	-10	6	621	622	4	-8	6	850	855	9	-6	6	599	635	-10	-3	6	853	[illegible]

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-8	-3	6	604	575	-12	-1	6	218	151	-6	-14	7	262	273	-3	-11	7	631	654	-9	-8	7	618	650
-7	-3	6	1969	1967	-11	-1	6	400	404	-5	-14	7	493	492	-2	-11	7	1280	1287	-8	-8	7	951	992
-6	-3	6	1223	1224	-10	-1	6	807	775	-4	-14	7	420	372	-1	-11	7	487	456	-7	-8	7	468	509
-5	-3	6	653	608	-8	-1	6	1252	1241	-2	-14	7	627	616	0	-11	7	566	539	-6	-8	7	710	729
-4	-3	6	1217	1225	[illegible]	-1	6	463	464	-1	-14	7	788	806	1	-11	7	248	239	-5	-8	7	380	369
-3	-3	6	841	902	-6	-1	6	1630	1590	0	-14	7	586	595	2	-11	7	1173	1184	-4	-8	7	543	543
-2	-3	6	645	677	-5	-1	6	454	416	1	-14	7	1335	1350	3	-11	7	1121	1179	-3	-8	7	1231	1226
-1	-3	6	1343	1359	-4	-1	6	904	918	2	-14	7	294	264	4	-11	7	817	790	-2	-8	7	402	390
0	-3	6	2312	2369	-3	-1	6	1649	1687	3	-14	7	534	481	5	-11	7	677	647	-1	-8	7	1174	1186
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2	-3	6	1783	1825	-1	-1	6	1849	1873	-10	-13	7	285	230	-11	-10	7	424	379	1	-8	7	477	448
3	-3	6	724	745	0	-1	6	423	404	-9	-13	7	723	750	-9	-10	7	256	318	2	-8	7	678	639
4	-3	6	295	256	1	-1	6	998	1068	-8	-13	7	480	488	-8	-10	7	1230	1314	3	-8	7	436	438
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6	-3	6	1057	1093	4	-1	6	359	363	-5	-13	7	648	628	-4	-10	7	1389	1445	6	-8	7	662	657
7	-3	6	385	382	6	-1	6	1088	1101	-4	-13	7	783	803	-3	-10	7	735	751	-15	-7	7	339	331
8	-3	6	817	876	8	-1	6	585	590	-3	-13	7	355	346	-2	-10	7	1463	1478	-14	-7	7	321	275
9	-3	6	745	771	9	-1	6	997	1045	-1	-13	7	1088	1083	-1	-10	7	694	690	-13	-7	7	693	708
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-14	-2	6	365	400	-14	0	6	964	971	4	-13	7	499	532	5	-10	7	300	229	-8	-7	7	691	692
-13	-2	6	815	804	-12	0	6	842	832	-12	-12	7	624	654	6	-10	7	392	362	-7	-7	7	851	861
-12	-2	6	1248	1221	-10	0	6	1445	1383	-10	-12	7	238	188	7	-10	7	240	289	-6	-7	7	2111	2211
-10	-2	6	369	350	-8	0	6	3079	3043	-9	-12	7	491	512	-14	-9	7	1120	1131	-4	-7	7	1731	1771
-9	-2	6	1988	1932	-6	0	6	392	372	-8	-12	7	433	476	-12	-9	7	272	327	-2	-7	7	482	475
-8	-2	6	516	479	-4	0	6	1225	1198	-7	-12	7	722	767	-11	-9	7	281	367	-1	-7	7	664	679
-7	-2	6	2168	2145	-2	0	6	609	649	-6	-12	7	765	767	-10	-9	7	1528	1630	0	-7	7	828	856
-6	-2	6	1559	1539	0	0	6	666	730	-5	-12	7	537	562	-9	-9	7	801	853	1	-7	7	241	267
-5	-2	6	165	97	2	0	6	823	900	-4	-12	7	283	307	-8	-9	7	1655	1698	2	-7	7	507	466
-4	-2	6	1546	1598	4	0	6	2176	2177	-3	-12	7	1266	1293	-7	-9	7	817	875	3	-7	7	1090	1120
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-2	-2	6	709	759	8	0	6	538	555	-1	-12	7	397	408	-5	-9	7	744	777	5	-7	7	579	599
-1	-2	6	325	299	10	0	6	443	432	0	-12	7	911	933	-3	-9	7	581	609	6	-7	7	1632	1654
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6	-2	6	890	892	-4	-15	7	293	255	-11	-11	7	339	331	5	-9	7	564	533	-11	-6	7	1432	1468
7	-2	6	386	413	-3	-15	7	312	318	-10	-11	7	576	613	7	-9	7	307	322	-10	-6	7	538	532
8	-2	6	1314	1373	-2	-15	7	434	452	-9	-11	7	1457	1500	-15	-8	7	777	829	-7	-6	7	1607	1624
-17	-1	6	413	371	-1	-15	7	543	518	-8	-11	7	678	708	-14	-8	7	448	437	-5	-6	7	643	655
-16	-1	6	998	993	0	-15	7	294	305	-7	-11	7	722	706	-13	-8	7	574	552	-3	-6	7	388	406
-15	-1	6	1015	984	1	-15	7	365	312	-6	-11	7	395	424	-12	-8	7	773	827	-2	-6	7	563	576
-14	-1	6	1715	1693	-8	-14	7	260	270	-5	-11	7	195	233	-11	-8	7	543	595	-1	-6	7	1221	1230
-13	-1	6	1097	1067	-7	-14	7	906	914	-4	-11	7	190	105	-10	-8	7	352	360	0	-6	7	1759	1789

H3OEP+ RE2(CO)6CL3-   MO DATA   0-40 DEG IN 2THETA   10 FO AND 10FC   PAGE 12

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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2	-6	7	1314	1383	-13	-3	7	897	908	-13	-1	7	527	548	-3	-13	8	588	576	-10	-9	8	408	414
3	-6	7	354	338	-12	-3	7	506	481	-12	-1	7	522	515	-2	-13	8	770	749	-9	-9	8	705	687
4	-6	7	299	262	-9	-3	7	1088	1091	-11	-1	7	674	669	-1	-13	8	601	593	-8	-9	8	1558	1547
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7	-6	7	486	496	-5	-3	7	1276	1286	-8	-1	7	1130	1107	2	-13	8	505	499	-4	-9	8	1294	1295
9	-6	7	424	440	-4	-3	7	1046	1069	-7	-1	7	840	824	-11	-12	8	669	693	-3	-9	8	246	274
-13	-5	7	1003	1015	-3	-3	7	670	694	-6	-1	7	699	693	-10	-12	8	352	425	-2	-9	8	1042	1058
-11	-5	7	304	301	-2	-3	7	188	139	-5	-1	7	263	247	-9	-12	8	721	758	-1	-9	8	579	563
-8	-5	7	464	476	-1	-3	7	2312	2417	-4	-1	7	336	353	-8	-12	8	383	392	0	-9	8	232	197
-7	-5	7	1820	1884	0	-3	7	1088	1131	-3	-1	7	382	386	-6	-12	8	1013	995	1	-9	8	828	831
-6	-5	7	490	507	2	-3	7	286	294	-2	-1	7	1762	1755	-4	-12	8	311	328	2	-9	8	416	414
-5	-5	7	2499	2554	3	-3	7	926	977	-1	-1	7	672	671	-3	-12	8	937	962	3	-9	8	600	571
-3	-5	7	324	360	4	-3	7	832	837	0	-1	7	882	926	-2	-12	8	445	393	4	-9	8	1041	1042
-2	-5	7	365	385	6	-3	7	1382	1434	1	-1	7	534	577	-1	-12	8	763	794	5	-9	8	628	577
-1	-5	7	1576	1681	7	-3	7	829	868	2	-1	7	846	884	1	-12	8	483	497	-14	-8	8	542	542
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9	-5	7	895	938	-13	-2	7	932	930	8	-1	7	425	465	-7	-11	8	656	646	-6	-8	8	963	950
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-14	-4	7	392	389	-11	-2	7	200	170	10	-1	7	373	349	-4	-11	8	789	799	-3	-8	8	801	869
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-12	-4	7	1148	1142	-9	-2	7	736	726	-14	0	7	1597	1553	-1	-11	8	525	550	-1	-8	8	401	378
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-4	-4	7	624	606	-3	-2	7	2684	2744	0	0	7	781	792	-12	-10	8	219	160	6	-8	8	773	762
-3	-4	7	693	750	-2	-2	7	295	297	2	0	7	287	298	-10	-10	8	1081	1042	-15	-7	8	536	531
-2	-4	7	1347	1410	-1	-2	7	1770	1811	4	0	7	967	901	-9	-10	8	385	398	-14	-7	8	668	652
-1	-4	7	825	875	0	-2	7	1760	1802	8	0	7	1188	1240	-8	-10	8	847	863	-12	-7	8	1258	1270
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3	-4	7	349	386	4	-2	7	384	406	-6	-14	8	253	236	-1	-10	8	363	398	-7	-7	8	931	932
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7	-4	7	325	337	7	-2	7	453	494	-1	-14	8	547	522	3	-10	8	279	322	-3	-7	8	1033	1048
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-16	-3	7	454	436	-17	-1	7	271	206	-7	-13	8	566	607	-13	-9	8	567	511	2	-7	8	979	1013
-15	-3	7	555	549	-15	-1	7	399	337	-5	-13	8	458	483	-12	-9	8	216	164	3	-7	8	312	313

H3OEP+ RE2(CO)6CL3- MO DATA 0-40 DEG IN 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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6	-7	8	525	383	4	-4	8	954	905	-16	-1	8	978	931	1	-12	9	311	288	3	-8	9	898	877
7	-7	8	419	422	5	-4	8	1340	1355	-15	-1	8	641	618	-11	-11	9	728	747	4	-8	9	516	515
-15	-6	8	320	301	6	-4	8	876	870	-14	-1	8	270	287	-10	-11	9	390	469	5	-8	9	782	767
-13	-6	8	379	365	7	-4	8	1502	1617	-13	-1	8	361	344	-9	-11	9	369	395	-12	-7	9	652	667
-11	-6	8	460	481	8	-4	8	448	446	-12	-1	8	485	500	-7	-11	9	381	425	-11	-7	9	522	541
-9	-6	8	356	374	-15	-3	8	524	527	-11	-1	8	289	226	-6	-11	9	326	318	-10	-7	9	318	302
-8	-6	8	902	877	-14	-3	8	549	566	-10	-1	8	508	523	-5	-11	9	459	454	-9	-7	9	738	705
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-2	-6	8	180	202	-8	-3	8	230	263	-3	-1	8	785	845	1	-11	9	303	316	-3	-7	9	778	778
-1	-6	8	1100	1090	-7	-3	8	747	752	-2	-1	8	889	899	2	-11	9	566	570	-1	-7	9	750	749
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-14	-5	8	268	252	1	-3	8	876	912	7	-1	8	443	479	2	-10	9	1017	1013	-12	-6	9	893	875
-13	-5	8	1157	1115	2	-3	8	1271	1302	8	-1	8	947	1009	-12	-9	9	499	496	-11	-6	9	310	336
-11	-5	8	1581	1535	3	-3	8	477	504	-16	0	8	920	871	-10	-9	9	919	932	-10	-6	9	230	205
-9	-5	8	400	391	4	-3	8	254	283	-14	0	8	1604	1527	-9	-9	9	320	293	-9	-6	9	559	575
-7	-5	8	642	640	5	-3	8	914	919	-10	0	8	2209	2157	-7	-9	9	572	544	-8	-6	9	287	294
-5	-5	8	621	617	6	-3	8	335	348	-8	0	8	1025	972	-5	-9	9	470	444	-7	-6	9	299	198
-4	-5	8	283	311	-15	-2	8	1001	959	-6	0	8	691	673	-4	-9	9	1050	1116	-6	-6	9	314	343
-2	-5	8	306	241	-14	-2	8	419	416	-4	0	8	1264	1277	-3	-9	9	346	349	-5	-6	9	710	724
-1	-5	8	2089	2153	-13	-2	8	882	872	-2	0	8	1925	1886	-2	-9	9	1140	1143	-4	-6	9	296	210
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2	-5	8	288	275	-9	-2	8	1719	1674	4	0	8	963	985	-14	-8	9	407	370	0	-6	9	1416	1456
5	-5	8	573	577	-8	-2	8	691	684	8	0	8	250	245	-13	-8	9	412	405	1	-6	9	714	731
-16	-4	8	294	234	-7	-2	8	690	664	-8	-13	9	620	626	-12	-8	9	645	669	2	-6	9	842	865
-15	-4	8	467	445	-6	-2	8	1323	1335	-7	-13	9	643	667	-11	-8	9	705	706	-15	-5	9	226	220
-13	-4	8	475	476	-5	-2	8	516	549	-6	-13	9	745	767	-10	-8	9	351	349	-14	-5	9	246	190
-11	-4	8	555	545	-4	-2	8	396	365	-4	-13	9	622	602	-9	-8	9	1036	1036	-13	-5	9	397	397
-9	-4	8	261	236	-3	-2	8	1187	1214	-3	-13	9	753	735	-8	-8	9	773	801	-12	-5	9	222	162
-8	-4	8	617	619	-2	-2	8	1153	1197	-1	-13	9	326	362	-7	-8	9	520	514	-11	-5	9	845	864
-7	-4	8	1651	1624	-1	-2	8	1540	1560	-9	-12	9	917	922	-6	-8	9	454	459	-9	-5	9	453	440
-6	-4	8	981	1004	0	-2	8	529	520	-8	-12	9	460	465	-5	-8	9	303	304	-7	-5	9	1846	1876
-5	-4	8	1334	1364	2	-2	8	609	594	-7	-12	9	393	346	-4	-8	9	735	737	-5	-5	9	1646	1080
-4	-4	8	776	754	3	-2	8	1151	1182	-6	-12	9	231	256	-3	-8	9	630	624	-4	-5	9	362	301
-3	-4	8	775	792	5	-2	8	685	760	-5	-12	9	699	722	-2	-8	9	312	297	-3	-5	9	609	660
-2	-4	8	251	248	6	-2	8	1320	1367	-3	-12	9	622	595	-1	-8	9	530	572	-2	-5	9	421	445
-1	-4	8	1128	1157	7	-2	8	327	333	-2	-12	9	442	464	0	-8	9	894	894	-1	-5	9	229	210

H3OEP+ RE2(CO)6CL3-   MO DATA   0-40 DEG IN 2THETA   10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
1	-5	9	616	646	-5	-2	9	778	807	-4	-11	10	345	347	-12	-6	10	637	638	-5	-3	10	443	439
2	-5	9	256	233	-4	-2	9	618	643	-2	-11	10	330	327	-11	-6	10	853	853	-4	-3	10	309	268
5	-5	9	1326	1325	-3	-2	9	717	706	-10	-10	10	256	276	-8	-6	10	594	586	-3	-3	10	223	177
-15	-4	9	270	224	-2	-2	9	1076	1131	-8	-10	10	268	288	-7	-6	10	970	961	-2	-3	10	1155	1119
-14	-4	9	346	318	-1	-2	9	341	393	-4	-10	10	1430	1444	-6	-6	10	818	818	-1	-3	10	869	882
-13	-4	9	1178	1207	0	-2	9	1348	1390	-2	-10	10	1086	1038	-4	-6	10	415	400	0	-3	10	1069	1121
-12	-4	9	467	454	1	-2	9	732	713	0	-10	10	233	206	-3	-6	10	570	568	2	-3	10	448	453
-11	-4	9	549	558	3	-2	9	1081	1055	1	-10	10	247	244	-1	-6	10	270	237	3	-3	10	866	906
-10	-4	9	343	343	4	-2	9	294	289	-12	-9	10	260	183	0	-6	10	803	798	5	-3	10	416	408
-9	-4	9	629	674	5	-2	9	281	249	-11	-9	10	393	417	1	-6	10	453	451	-15	-2	10	836	788
-8	-4	9	328	351	-16	-1	9	852	816	-10	-9	10	1134	1118	3	-6	10	361	297	-12	-2	10	83[illegible]	810
-6	-4	9	271	254	-15	-1	9	598	571	-9	-9	10	414	395	4	-6	10	639	613	-11	-2	10	761	751
-5	-4	9	935	963	-14	-1	9	793	746	-8	-9	10	849	866	-13	-5	10	1018	984	-10	-2	10	309	292
-4	-4	9	206	202	-13	-1	9	346	342	-7	-9	10	202	96	-11	-5	10	285	275	-9	-2	10	482	487
-3	-4	9	288	319	-12	-1	9	626	603	-6	-9	10	420	387	-9	-5	10	294	286	-8	-2	10	901	898
-2	-4	9	623	599	-11	-1	9	477	474	-4	-9	10	731	727	-7	-5	10	622	628	-7	-2	10	476	471
-1	-4	9	2105	2126	-10	-1	9	1230	1161	-1	-9	10	361	361	-5	-5	10	1032	1065	-6	-2	10	256	235
0	-4	9	941	989	-9	-1	9	867	838	1	-9	10	432	421	-3	-5	10	669	687	-5	-2	10	1128	1129
1	-4	9	1310	1368	-8	-1	9	420	413	2	-9	10	1009	1023	-2	-5	10	323	324	-4	-2	10	434	450
2	-4	9	525	498	-7	-1	9	613	594	-12	-8	10	678	675	-1	-5	10	1834	1825	-3	-2	10	1316	1342
3	-4	9	477	496	-5	-1	9	791	764	-10	-8	10	465	486	0	-5	10	262	290	-2	-2	10	204	178
5	-4	9	293	340	-4	-1	9	1474	1475	-8	-8	10	356	357	1	-5	10	614	625	-1	-2	10	441	386
-15	-3	9	845	801	-3	-1	9	1084	1134	-7	-8	10	203	191	3	-5	10	378	347	0	-2	10	601	563
-12	-3	9	346	336	-2	-1	9	1636	1687	-6	-8	10	373	317	-14	-4	10	267	305	1	-2	10	690	720
-11	-3	9	1006	1028	-1	-1	9	659	670	-5	-8	10	781	792	-13	-4	10	721	663	2	-2	10	367	338
-9	-3	9	639	598	0	-1	9	214	246	-4	-8	10	477	491	-12	-4	10	227	264	3	-2	10	434	438
-8	-3	9	1258	1233	1	-1	9	348	344	-3	-8	10	1152	1128	-11	-4	10	973	937	4	-2	10	626	628
-7	-3	9	490	507	2	-1	9	841	895	-2	-8	10	240	202	-9	-4	10	483	448	-14	-1	10	397	369
-6	-3	9	1540	1551	3	-1	9	568	622	-1	-8	10	584	548	-8	-4	10	625	593	-11	-1	10	763	726
-5	-3	9	195	138	5	-1	9	240	258	0	-8	10	574	530	-7	-4	10	1306	1296	-10	-1	10	1269	1234
-4	-3	9	323	340	7	-1	9	410	440	2	-8	10	259	267	-6	-4	10	921	894	-9	-1	10	966	950
-3	-3	9	1672	1689	-16	0	9	706	682	-12	-7	10	577	586	-5	-4	10	222	214	-8	-1	10	900	868
-2	-3	9	325	347	-10	0	9	1183	1147	-11	-7	10	360	361	-4	-4	10	288	271	-7	-1	10	675	657
-1	-3	9	734	750	-8	0	9	1859	1827	-9	-7	10	854	879	-3	-4	10	627	672	-6	-1	10	298	262
0	-3	9	310	296	-6	0	9	241	316	-8	-7	10	220	205	-2	-4	10	491	464	-5	-1	10	296	287
1	-3	9	804	828	-4	0	9	1451	1428	-7	-7	10	268	243	-1	-4	10	441	442	-4	-1	10	218	228
4	-3	9	786	816	-2	0	9	402	412	-6	-7	10	679	694	1	-4	10	856	879	-2	-1	10	410	409
6	-3	9	1242	1264	2	0	9	1186	1235	-5	-7	10	610	626	4	-4	10	724	763	-1	-1	10	399	378
-15	-2	9	316	338	4	0	9	1284	1289	-3	-7	10	211	225	5	-4	10	1069	1087	1	-1	10	638	693
-14	-2	9	719	674	-6	-12	10	417	425	-2	-7	10	1119	1120	-15	-3	10	259	193	2	-1	10	1005	1003
-12	-2	9	625	600	-5	-12	10	555	544	-1	-7	10	227	251	-14	-3	10	588	561	3	-1	10	674	690
-11	-2	9	558	516	-4	-12	10	275	289	0	-7	10	1030	1047	-13	-3	10	466	459	4	-1	10	912	940
-10	-2	9	401	363	-3	-12	10	1063	1038	1	-7	10	449	466	-12	-3	10	538	498	5	-1	10	394	390
-9	-2	9	1208	1231	-9	-11	10	877	889	2	-7	10	268	324	-11	-3	10	633	607	-14	0	10	566	589
-8	-2	9	659	677	-8	-11	10	270	261	3	-7	10	710	704	-9	-3	10	1037	962	-12	0	10	668	639
-7	-2	9	796	797	-6	-11	10	551	563	-14	-6	10	407	435	-8	-3	10	391	4[illegible]1	-10	0	10	711	696
-6	-2	9	582	593	-5	-11	10	236	281	-13	-6	10	493	449	-6	-3	10	1052	1032	-8	0	10	226	177

H3OEP+ RE2(CO)6CL3- MD DATA 0-40 DEG IN 2THETA 10 FO AND 10FC PAGE 15

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-6	0	10	462	446	1	-5	11	721	719	-4	-1	11	1247	1246	-9	-2	12	292	260					
-4	0	10	2065	2032	-13	-4	11	266	261	-3	-1	11	641	681	-8	-2	12	538	520					
-2	0	10	1468	1444	-12	-4	11	307	313	-2	-1	11	484	452	-7	-2	12	292	286					
0	0	10	217	235	-11	-4	11	405	392	-1	-1	11	267	219	-5	-2	12	753	712					
2	0	10	390	920	-10	-4	11	438	433	0	-1	11	487	501	-4	-2	12	480	468					
4	0	10	340	356	-8	-4	11	541	516	1	-1	11	280	262	-3	-2	12	615	603					
-6	-10	11	278	323	-7	-4	11	904	878	-14	0	11	290	272	-2	-2	12	548	496					
-8	-9	11	295	276	-6	-4	11	394	389	-12	0	11	783	739	0	-2	12	384	408					
-7	-9	11	417	411	-5	-4	11	610	622	-10	0	11	1551	1469	-12	-1	12	657	632					
-6	-9	11	450	436	-3	-4	11	804	800	-8	0	11	824	795	-11	-1	12	661	637					
-5	-9	11	513	554	-2	-4	11	428	464	-6	0	11	349	389	-10	-1	12	791	700					
-4	-9	11	1080	1053	-1	-4	11	1106	1108	0	0	11	1015	1062	-9	-1	12	525	509					
-3	-9	11	694	718	0	-4	11	368	377	2	0	11	1330	1310	-7	-1	12	382	364					
-2	-9	11	402	376	2	-4	11	513	492	-8	-7	12	679	711	-6	-1	12	312	293					
-1	-9	11	477	474	-13	-3	11	645	590	-7	-7	12	241	239	-4	-1	12	266	276					
-11	-8	11	376	368	-12	-3	11	607	583	-6	-7	12	725	748	-2	-1	12	242	215					
-10	-8	11	403	389	-11	-3	11	344	329	-9	-6	12	404	403	-1	-1	12	346	375					
-9	-8	11	540	553	-9	-3	11	340	353	-8	-6	12	470	437	0	-1	12	650	647					
-6	-8	11	493	493	-8	-3	11	657	676	-6	-6	12	329	370	-10	0	12	505	466					
-2	-8	11	472	492	-7	-3	11	487	507	-5	-6	12	378	422	-6	0	12	627	615					
-1	-8	11	225	253	-6	-3	11	454	465	-4	-6	12	208	218	-4	0	12	1163	1124					
-8	-7	11	765	760	-5	-3	11	713	721	-2	-6	12	510	465	-2	0	12	263	262					
-7	-7	11	230	142	-4	-3	11	247	254	-9	-5	12	610	616	-6	-2	13	267	291					
-6	-7	11	380	366	-3	-3	11	671	690	-7	-5	12	1146	1107	-7	-1	13	321	331					
-5	-7	11	539	562	-2	-3	11	475	440	-5	-5	12	406	430	-6	-1	13	711	712					
-3	-7	11	878	852	0	-3	11	869	858	-3	-5	12	591	608	-5	-1	13	471	463					
-2	-7	11	541	499	1	-3	11	455	457	-1	-5	12	459	476	-6	0	13	254	161					
0	-7	11	1022	981	3	-3	11	506	501	-9	-4	12	685	663										
-11	-6	11	314	259	-14	-2	11	550	503	-7	-4	12	318	322										
-8	-6	11	441	429	-13	-2	11	239	202	-5	-4	12	505	517										
-7	-6	11	662	620	-12	-2	11	262	259	-4	-4	12	247	252										
-6	-6	11	766	789	-11	-2	11	1110	1047	-3	-4	12	217	167										
-5	-6	11	582	566	-10	-2	11	401	378	-2	-4	12	410	395										
-3	-6	11	307	286	-9	-2	11	1081	1015	-1	-4	12	742	761										
-2	-6	11	556	567	-7	-2	11	216	119	-11	-3	12	669	683										
-1	-6	11	607	624	-6	-2	11	888	845	-10	-3	12	411	360										
0	-6	11	315	359	-3	-2	11	207	177	-9	-3	12	247	218										
1	-6	11	256	239	-2	-2	11	886	869	-8	-3	12	877	854										
-13	-5	11	1093	1067	-1	-2	11	339	338	-7	-3	12	537	477										
-11	-5	11	571	574	0	-2	11	337	349	-6	-3	12	906	897										
[illegible]	-5	11	733	731	1	-2	11	1271	1244	-5	-3	12	335	432										
[illegible]	[illegible]	11	410	409	2	-2	11	611	641	-4	-3	12	211	254										
[illegible]	[illegible]	11	375	888	3	-2	11	952	949	-3	-3	12	458	454										
[illegible]	[illegible]	11	261	205	-12	-1	11	549	545	-2	-3	12	391	416										
[illegible]	[illegible]	11	[illegible]	236	-8	-1	11	458	483	-12	-2	12	411	439										
[illegible]	[illegible]	11	[illegible]	1187	-6	-1	11	448	408	-11	-2	12	268	201										
[illegible]	[illegible]	11	[illegible]	226	-5	-1	11	694	665	-10	-2	12	275	209										

H3OEP+ RE2(CO)6CL3- MO DATA 40-55 DEG 2THETA 10 FO AND 10FC

H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC
1-25	0	279	195	14-15	0	233	251	2-25	1	296	268	-14-19	1	420	482	-17-15	1	326	379
3-25	0	416	380	15-15	0	809	768	3-25	1	423	403	-12-19	1	645	656	-11-15	1	730	772
3-24	0	384	384	16-15	0	308	247	4-25	1	385	319	-11-19	1	237	224	15-15	1	578	559
5-24	0	334	338	12-14	0	558	534	-3-24	1	649	624	-9-19	1	372	374	16-15	1	286	214
7-24	0	302	290	14-14	0	286	255	1-24	1	419	417	6-19	1	341	378	17-15	1	327	297
3-23	0	457	443	15-14	0	478	453	3-24	1	315	332	-5-19	1	395	377	-17-14	1	467	485
4-23	0	406	334	17-14	0	449	437	6-24	1	285	290	-4-19	1	319	297	-15-14	1	651	934
6-23	0	354	349	13-13	0	490	455	-10-23	1	[illegible]	282	-3-19	1	373	366	-14-14	1	230	209
7-23	0	269	250	14-13	0	427	423	-9-23	1	[illegible]	372	-2-19	1	903	878	11-14	1	547	493
8-23	0	276	286	15-13	0	531	525	-8-23	1	293	294	1-19	1	362	358	13-14	1	626	619
1-22	0	611	600	16-13	0	502	534	-5-23	1	443	449	2-19	1	360	354	15-14	1	495	501
4-22	0	308	317	13-12	0	1230	1204	-1-23	1	377	409	3-19	1	377	333	-17-13	1	478	526
11-22	0	338	368	14-12	0	256	332	2-23	1	292	274	6-19	1	451	441	-16-13	1	312	251
2-21	0	275	280	16-12	0	524	521	3-23	1	379	328	8-19	1	489	504	-14-13	1	412	483
5-21	0	787	778	14-11	0	701	689	4-23	1	334	291	10-19	1	369	386	-13-13	1	620	653
6-21	0	420	417	17-11	0	410	361	7-23	1	356	328	12-19	1	760	733	12-13	1	630	615
7-21	0	766	735	18-11	0	450	475	-7-22	1	631	637	-16-18	1	282	325	13-13	1	303	253
0-20	0	1035	1043	19-11	0	455	423	-5-22	1	326	351	-12-18	1	364	310	14-13	1	665	661
1-20	0	507	473	14-10	0	814	748	-4-22	1	457	453	-10-18	1	324	271	15-13	1	524	578
2-20	0	534	528	16-10	0	442	425	-2-22	1	377	385	-9-18	1	253	161	16-13	1	317	337
5-20	0	322	286	15 -9	0	250	228	1-22	1	347	341	-8-18	1	717	761	17-13	1	312	252
8-20	0	327	255	17 -9	0	570	502	2-22	1	254	284	-7-18	1	490	507	-19-12	1	445	518
11-20	0	304	207	18 -9	0	653	646	4-22	1	297	251	-6-18	1	607	679	-16-12	1	539	628
12-20	0	682	629	15 -8	0	313	325	5-22	1	688	649	5-18	1	785	729	-14-12	1	580	637
2-19	0	290	331	16 -8	0	445	413	7-22	1	411	402	6-18	1	975	929	13-12	1	413	331
3-19	0	506	507	20 -8	0	289	336	-13-21	1	432	470	7-18	1	715	704	14-12	1	572	568
4-19	0	466	432	16 -7	0	820	740	-11-21	1	368	352	9-18	1	466	430	17-12	1	558	574
6-19	0	1217	1220	19 -7	0	404	375	-8-21	1	266	279	10-18	1	437	432	-18-11	1	507	516
8-19	0	463	487	16 -6	0	606	595	-5-21	1	384	353	14-18	1	450	326	-17-11	1	277	297
11-19	0	262	197	17 -6	0	570	541	-3-21	1	238	235	-16-17	1	262	199	-16-11	1	446	464
8-18	0	568	517	20 -6	0	349	345	-2-21	1	374	340	-13-17	1	463	441	-15-11	1	539	540
9-18	0	478	411	21 -6	0	401	411	-1-21	1	737	794	-12-17	1	262	208	-14-11	1	473	488
10-18	0	306	217	17 -5	0	435	436	0-21	1	364	388	-11-17	1	272	244	13-11	1	1171	1091
11-18	0	440	422	21 -5	0	383	362	1-21	1	565	513	-10-17	1	971	1006	15-11	1	362	336
12-18	0	432	410	16 -4	0	518	490	7-21	1	347	352	-8-17	1	797	831	16-11	1	362	368
13-18	0	391	344	17 -4	0	768	772	11-21	1	533	498	7-17	1	430	440	-20-10	1	554	582
9-17	0	326	345	20 -4	0	316	257	-8-20	1	465	493	8-17	1	895	881	-18-10	1	586	611
10-17	0	565	530	21 -4	0	599	615	-7-20	1	567	547	11-17	1	456	436	14-10	1	536	571
14-17	0	438	475	18 -3	0	307	245	-6-20	1	812	855	13-17	1	446	425	16-10	1	352	361
16-17	0	375	347	19 -3	0	428	460	-5-20	1	348	327	-16-16	1	577	575	18-10	1	822	804
9-16	0	688	682	17 -2	0	288	300	-3-20	1	291	298	-15-16	1	414	442	-18 -9	1	559	538
10-16	0	770	725	18 -2	0	353	261	0-20	1	313	266	-14-16	1	492	526	14 -9	1	519	499
15-16	0	302	246	20 -2	0	501	474	1-20	1	289	295	-11-16	1	353	350	15 -9	1	264	247
16-16	0	398	380	17 -1	0	708	755	4-20	1	845	820	-10-16	1	276	287	16 -9	1	257	218
17-16	0	297	222	18 -1	0	795	787	5-20	1	672	635	9-16	1	496	508	17 -9	1	266	203
11-15	0	581	515	19 -1	0	550	545	6-20	1	932	908	10-16	1	931	902	-21 -8	1	270	238
13-15	0	287	320	20 -1	0	370	322	7-20	1	448	446	14-16	1	428	415	-20 -9	1	327	265

H3OEP+ RE2(CO)6CL3- MO DATA 40-55 DEG 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-19	-8	1	446	475	-18	0	1	633	685	6	-20	2	512	525	14	-16	2	511	492	14	-9	2	578	567
-17	-9	1	256	284	18	0	1	1106	1070	7	-20	2	256	223	16	-16	2	428	371	16	-9	2	484	479
-16	-8	1	634	684	-5	-25	2	243	331	10	-20	2	440	496	-17	-15	2	623	631	17	-9	2	314	294
15	-8	1	270	271	-4	-25	2	439	411	11	-20	2	322	325	-16	-15	2	311	367	18	-9	2	337	545
17	-8	1	651	659	-3	-25	2	449	445	12	-20	2	507	481	-15	-15	2	672	728	-19	-8	2	374	422
16	-8	1	742	728	-2	-25	2	267	225	-12	-19	2	402	414	-12	-15	2	248	283	-18	-8	2	467	500
19	-8	1	411	415	1	-24	2	395	375	-8	-19	2	787	774	-11	-15	2	236	209	-17	-8	2	335	387
-20	-7	1	318	411	3	-24	2	668	603	-6	-19	2	590	626	9	-15	2	1253	1215	14	-8	2	415	371
-18	-7	1	244	315	-6	-23	2	367	326	-5	-19	2	476	460	10	-15	2	503	518	15	-8	2	410	377
-17	-7	1	448	453	-5	-23	2	246	266	-3	-19	2	633	642	11	-15	2	305	343	16	-8	2	275	306
-16	-7	1	602	597	-4	-23	2	372	367	-2	-19	2	220	218	13	-15	2	373	296	17	-8	2	390	321
16	-7	1	647	658	-3	-23	2	467	474	0	-19	2	556	593	-12	-14	2	446	525	19	-8	2	336	273
17	-7	1	263	226	-2	-23	2	375	340	1	-19	2	273	231	10	-14	2	513	534	-19	-7	2	281	228
20	-7	1	462	472	1	-23	2	474	373	4	-19	2	894	883	11	-14	2	321	338	-18	-7	2	397	418
-18	-6	1	329	385	5	-23	2	300	266	6	-19	2	759	751	12	-14	2	368	388	-16	-7	2	982	1019
-17	-6	1	624	622	4	-23	2	276	197	7	-19	2	334	311	13	-14	2	338	375	14	-7	2	683	728
-16	-6	1	753	830	-12	-22	2	345	273	9	-19	2	461	422	14	-14	2	272	261	17	-7	2	345	324
15	-6	1	713	676	-10	-22	2	452	440	12	-19	2	456	460	15	-14	2	649	641	-22	-6	2	447	466
16	-6	1	461	531	-7	-22	2	705	712	-14	-18	2	421	437	-18	-13	2	347	341	-21	-6	2	293	292
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-21	-5	1	725	746	-3	-22	2	396	401	-10	-18	2	491	521	-16	-13	2	727	756	-17	-6	2	443	445
-17	-5	1	714	729	-1	-22	2	572	604	-9	-18	2	343	350	-15	-13	2	573	642	15	-6	2	779	796
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-18	-4	1	395	461	4	-22	2	315	328	6	-18	2	591	620	13	-13	2	719	710	15	-5	2	580	550
-17	-4	1	608	622	5	-22	2	452	425	8	-18	2	497	508	17	-13	2	410	428	-21	-4	2	497	501
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21	-4	1	473	508	-7	-21	2	646	675	10	-18	2	371	341	-17	-12	2	308	365	-17	-4	2	601	618
-22	-3	1	497	502	-4	-21	2	228	196	11	-18	2	214	318	-15	-12	2	537	554	15	-4	2	1365	1393
-21	-3	1	769	753	-1	-21	2	465	464	12	-18	2	394	331	13	-12	2	511	460	16	-4	2	363	363
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-17	-3	1	455	458	3	-21	2	377	358	-14	-17	2	256	148	-20	-11	2	288	329	-19	-3	2	469	474
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20	-3	1	441	429	-14	-20	2	422	401	-8	-17	2	351	338	14	-11	2	320	345	20	-3	2	432	451
-19	-2	1	583	598	-13	-20	2	333	352	7	-17	2	444	412	16	-11	2	430	389	-22	-2	2	428	426
-17	-2	1	493	506	-12	-20	2	304	304	8	-17	2	709	758	17	-11	2	526	519	-19	-2	2	622	665
16	-2	1	267	228	-7	-20	2	296	395	10	-17	2	819	762	18	-11	2	362	338	-18	-2	2	574	539
17	-2	1	470	473	-6	-20	2	414	472	13	-17	2	290	269	-20	-10	2	287	343	-17	-2	2	370	388
18	-2	1	260	187	-5	-20	2	414	412	-13	-16	2	240	201	-18	-10	2	673	711	16	-2	2	661	711
19	-2	1	646	657	-3	-20	2	313	302	-12	-16	2	468	477	14	-10	2	252	222	19	-2	2	315	297
-19	-1	1	310	276	-2	-20	2	898	893	-11	-16	2	460	515	16	0	2	394	429	20	-2	2	285	286
-18	-1	1	520	518	-1	-20	2	577	540	-10	-16	2	960	983	-20	-9	2	394	443	-21	-1	2	260	282
20	-1	1	384	333	0	-20	2	789	766	8	-16	2	469	477	-19	-9	2	264	197	-20	-1	2	693	682
-20	0	1	701	673	4	-20	2	299	306	11	-16	2	297	205	-16	-9	2	521	397	-19	-1	2	366	338

H3OEP+ RE2(CO)6CL3- MO DATA 40-55 DEG 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
-18	-1	2	383	407	-1	-20	3	564	567	-17	-16	3	360	390	-20	-9	3	565	570	15	-1	3	490	468
-17	-1	2	574	581	0	-20	3	501	500	-16	-16	3	533	588	-19	-9	3	309	275	17	-1	3	416	482
16	-1	2	595	563	1	-20	3	318	299	-13	-16	3	300	287	-18	-9	3	535	580	18	-1	3	612	613
17	-1	2	444	494	4	-20	3	903	814	-11	-16	3	233	135	-16	-9	3	356	401	-22	0	3	313	241
18	-1	2	620	617	5	-20	3	270	217	7	-16	3	417	430	13	-9	3	360	408	-20	0	3	627	608
19	-1	2	497	476	10	-20	3	361	363	8	-16	3	1192	1161	15	-9	3	475	493	16	0	3	964	932
-20	0	2	600	545	-14	-19	3	405	434	9	-16	3	509	449	17	-9	3	311	216	18	0	3	474	459
-18	0	2	870	869	-11	-19	3	294	308	10	-16	3	552	575	19	-9	3	464	479	-3	-25	4	343	308
18	0	2	544	551	-9	-19	3	261	257	-15	-15	3	380	354	-21	-8	3	269	242	-3	-24	4	320	307
20	0	2	361	331	-8	-19	3	481	495	-11	-15	3	1370	1478	-18	-8	3	418	424	1	-24	4	562	557
1	-25	3	430	339	-6	-19	3	597	587	9	-15	3	321	295	-17	-8	3	336	347	3	-24	4	381	333
2	-25	3	342	311	-2	-19	3	1017	1020	13	-15	3	596	598	-16	-8	3	612	632	-5	-23	4	539	493
-5	-24	3	595	575	0	-19	3	352	336	14	-15	3	395	429	13	-8	3	569	575	-4	-23	4	449	435
-3	-24	3	507	513	1	-19	3	511	502	15	-15	3	465	459	15	-8	3	475	459	-2	-23	4	479	445
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-10	-23	3	369	340	4	-19	3	565	537	-15	-14	3	524	542	-22	-7	3	429	402	0	-23	4	320	316
-8	-23	3	284	292	6	-19	3	797	798	-14	-14	3	238	290	-19	-7	3	423	465	3	-23	4	299	332
-3	-23	3	298	267	10	-19	3	639	659	-13	-14	3	325	355	14	-7	3	1197	1186	-12	-22	4	273	302
0	-23	3	244	234	12	-19	3	476	417	9	-14	3	970	945	16	-7	3	663	656	-10	-22	4	331	333
1	-23	3	395	426	-15	-18	3	268	220	13	-14	3	427	408	17	-7	3	317	267	-7	-22	4	467	506
2	-23	3	[illegible]	314	-14	-18	3	266	279	-19	-13	3	417	445	-21	-6	3	301	291	-3	-22	4	757	371
-7	-22	3	274	294	-13	-18	3	337	303	-15	-13	3	480	514	-18	-6	3	472	470	0	-22	4	262	202
-6	-22	3	332	330	-12	-18	3	449	459	11	-13	3	727	741	-17	-6	3	984	1019	2	-22	4	378	380
-4	-22	3	520	492	-10	-18	3	237	175	12	-13	3	469	429	19	-6	3	378	340	3	-22	4	308	255
-2	-22	3	331	282	-8	-18	3	608	598	14	-13	3	573	585	-21	-5	3	380	363	5	-22	4	539	523
-1	-22	3	602	595	-7	-18	3	404	353	15	-13	3	334	373	-19	-5	3	249	195	-13	-21	4	426	461
1	-22	3	261	259	-6	-18	3	289	325	-18	-12	3	316	359	15	-5	3	1240	1243	-12	-21	4	260	150
3	-22	3	391	354	3	-18	3	345	332	-16	-12	3	583	599	-21	-4	3	451	427	-7	-21	4	271	204
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-13	-21	3	352	350	5	-18	3	515	520	-14	-12	3	263	250	-17	-4	3	1179	1185	-3	-21	4	589	606
-10	-21	3	255	177	6	-18	3	302	276	11	-12	3	900	943	17	-4	3	376	380	-1	-21	4	847	842
-9	-21	3	269	243	7	-18	3	540	533	12	-12	3	380	334	19	-4	3	371	330	3	-21	4	234	293
-7	-21	3	577	621	8	-18	3	434	428	13	-12	3	634	635	-22	-3	3	481	492	4	-21	4	334	213
-3	-21	3	456	463	9	-18	3	467	441	17	-12	3	498	501	-19	-3	3	775	760	-8	-20	4	561	563
-2	-21	3	384	427	11	-18	3	439	463	-20	-11	3	267	285	-18	-3	3	283	217	-7	-20	4	465	412
-1	-21	3	591	573	12	-18	3	450	403	-19	-11	3	387	407	15	-3	3	400	410	-6	-20	4	432	466
1	-21	3	248	227	-13	-17	3	322	239	-18	-11	3	443	452	16	-3	3	635	640	-4	-20	4	250	234
2	-21	3	262	246	-12	-17	3	505	554	-15	-11	3	516	576	17	-3	3	301	369	-3	-20	4	518	489
5	-21	3	663	649	-10	-17	3	1035	1065	12	-11	3	423	382	19	-3	3	405	427	-2	-20	4	405	436
7	-21	3	338	305	-8	-17	3	334	365	13	-11	3	421	416	-20	-2	3	301	298	2	-20	4	245	262
9	-21	3	379	379	5	-17	3	596	611	15	-11	3	273	234	-18	-2	3	406	422	4	-20	4	742	749
-13	-20	3	345	333	6	-17	3	286	326	17	-11	3	336	303	16	-2	3	382	387	5	-20	4	386	356
-12	-20	3	429	487	7	-17	3	261	276	-20	-10	3	379	423	17	-2	3	660	684	6	-20	4	567	577
-8	-20	3	541	520	10	-17	3	298	306	12	-10	3	1330	1333	20	-2	3	303	340	10	-20	4	425	452
-7	-20	3	297	232	11	-17	3	471	418	14	-10	3	327	323	-20	-1	3	636	636	-14	-19	4	568	557
-6	-20	3	375	347	14	-17	3	489	491	16	-10	3	481	473	-19	-1	3	611	596	-12	-19	4	463	466
-2	-20	3	433	403	-18	-15	3	352	366	18	-10	3	397	396	-18	-1	3	892	897	-10	-19	4	266	238

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H K	L	FOBS	FCALC
-9-19	4	259	245
-8-19	4	409	363
-5-19	4	461	524
-4-19	4	274	237
-3-19	4	309	314
-2-19	4	754	776
0-19	4	702	699
2-19	4	449	451
4-19	4	662	616
9-19	4	309	287
10-19	4	524	456
12-19	4	506	518
-16-18	4	274	329
-13-18	4	334	280
-12-18	4	459	452
-11-18	4	369	351
-10-18	4	413	413
-9-18	4	455	486
-8-18	4	455	464
-7-18	4	388	421
-6-18	4	416	441
1-18	4	473	478
2-18	4	611	605
3-18	4	770	717
5-18	4	675	681
6-18	4	340	345
8-18	4	306	201
10-18	4	464	452
11-18	4	288	280
-16-17	4	335	335
-13-17	4	411	416
-10-17	4	506	527
-9-17	4	246	261
-8-17	4	338	311
4-17	4	319	337
5-17	4	387	367
6-17	4	378	413
7-17	4	246	199
8-17	4	836	812
9-17	4	275	307
11-17	4	430	456
-16-16	4	301	330
-15-16	4	266	300
-12-16	4	689	706
-11-16	4	711	796
-10-16	4	802	802
8-16	4	384	363

H K	L	FOBS	FCALC
9-16	4	336	289
10-16	4	304	288
12-16	4	326	264
14-16	4	591	568
-19-15	4	343	264
-18-15	4	290	211
-17-15	4	494	547
-13-15	4	237	221
-11-15	4	344	345
7-15	4	980	923
8-15	4	570	563
9-15	4	656	630
15-15	4	298	191
-17-14	4	257	244
-15-14	4	403	456
-13-14	4	500	540
-12-14	4	255	243
8-14	4	260	218
9-14	4	957	934
13-14	4	603	610
15-14	4	428	430
-17-13	4	449	451
-16-13	4	494	526
-14-13	4	328	340
-13-13	4	663	737
10-13	4	407	415
11-13	4	716	706
15-13	4	304	317
-19-12	4	604	634
-15-12	4	502	548
10-12	4	462	456
11-12	4	531	555
12-12	4	374	356
14-12	4	492	454
-18-11	4	305	309
-15-11	4	661	694
11-11	4	848	826
12-11	4	861	929
13-11	4	378	410
15-11	4	309	269
16-11	4	325	363
-20-10	4	646	689
-18-10	4	548	570
-16-10	4	351	382
-15-10	4	307	313
12-10	4	388	377
16-10	4	563	562

H K	L	FOBS	FCALC
-18 -9	4	329	326
-17 -9	4	368	349
-16 -9	4	256	230
12 -9	4	830	846
13	4	341	335
16 -	4	467	459
-21 -8	4	374	362
-20 -8	4	340	413
-19 -8	4	476	521
-16 -8	4	658	684
12 -8	4	273	230
13 -8	4	469	429
14 -8	4	486	460
15 -8	4	389	426
17 -8	4	505	473
-22 -7	4	342	296
-18 -7	4	793	840
13 -7	4	342	402
16 -7	4	396	349
-22 -6	4	298	313
-17 -6	4	333	253
13 -6	4	545	518
14 -6	4	900	924
15 -6	4	425	385
16 -6	4	293	384
-21 -5	4	269	332
-19 -5	4	374	397
-17 -5	4	1322	1359
15 -5	4	495	519
-22 -4	4	289	263
-20 -4	4	364	312
-19 -	4	271	305
14 -4	4	460	412
15 -4	4	725	743
16 -4	4	309	315
-22 -3	4	274	257
-21 -3	4	329	285
-18 -3	4	687	747
14 -3	4	467	472
15 -3	4	613	693
17 -3	4	410	415
-21 -2	4	581	554
-20 -2	4	350	332
-19 -2	4	875	875
-18 -2	4	251	240
14 -2	4	916	952
15 -2	4	487	429

H K	L	FOBS	FCALC
17 -2	4	762	804
18 -2	4	363	268
19 -2	4	374	292
-22 -1	4	296	329
-18 -1	4	289	373
16 -1	4	533	561
-22 0	4	424	379
-20 0	4	1011	1080
-18 0	4	549	957
16 0	4	788	835
18 0	4	811	862
-7-24	5	293	266
-5-24	5	531	541
-2-24	5	327	245
1-24	5	267	230
-3-23	5	379	302
1-23	5	467	445
4-23	5	383	315
-6-22	5	414	383
-4-22	5	413	403
-3-22	5	449	459
-2-22	5	325	275
-1-22	5	537	529
0-22	5	251	233
6-22	5	276	194
-9-21	5	444	507
-8-21	5	267	247
-7-21	5	577	564
-3-21	5	260	175
0-21	5	246	240
3-21	5	564	519
4-21	5	266	208
5-21	5	672	657
-14-20	5	476	479
-13-20	5	279	237
-12-20	5	267	280
-9-20	5	255	196
-4-20	5	313	331
-3-20	5	490	475
-2-20	5	825	799
-1-20	5	588	579
0-20	5	423	364
2-20	5	348	332
3-20	5	335	328
-11-19	5	273	255
-10-19	5	286	265
-8-19	5	786	798

H K	L	FOBS	FCALC
-6-19	5	428	437
-5-19	5	237	213
-4-19	5	395	380
-3-19	5	228	239
0-19	5	397	361
1-19	5	317	333
3-19	5	268	252
4-19	5	888	896
6-19	5	466	456
8-19	5	293	271
-14-18	5	505	497
-13-18	5	414	404
-11-18	5	364	381
-10-18	5	590	602
-6-18	5	418	410
-5-18	5	292	318
-3-18	5	638	642
-2-18	5	703	686
-1-18	5	552	574
0-18	5	319	301
2-18	5	625	657
4-18	5	365	384
6-18	5	330	315
7-18	5	366	372
9-18	5	384	452
10-18	5	370	294
11-18	5	411	386
-16-17	5	389	419
-12-17	5	769	824
-10-17	5	594	545
-9-17	5	355	376
-7-17	5	467	47
2-17	5	961	[illegible]
3-17	5	571	552
5-17	5	537	508
6-17	5	276	166
8-17	5	544	545
9-17	5	313	294
12-17	5	361	381
-18-16	5	285	316
-12-16	5	404	440
-11-16	5	385	436
-10-16	5	683	730
-9-16	5	378	370
4-16	5	373	344
5-16	5	239	212
6-16	5	660	654

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H K	L	FOBS	FCALC
7-16	5	335	317
8-16	5	672	648
10-16	5	285	223
-17-15	5	426	421
-13-15	5	734	795
-12-15	5	373	370
-11-15	5	1057	1105
7-15	5	546	527
8-15	5	316	306
9-15	5	646	582
10-15	5	278	221
13-15	5	543	488
14-15	5	289	306
-19-14	5	329	318
-17-14	5	363	385
-12-14	5	301	322
7-14	5	950	921
10-14	5	392	375
11-14	5	287	270
12-14	5	315	271
13-14	5	293	246
-19-13	5	303	352
-16-13	5	287	255
-13-13	5	537	553
8-13	5	427	450
9-13	5	750	701
12-13	5	462	472
13-13	5	438	447
14-13	5	426	332
-19-12	5	262	154
-15-12	5	772	773
9-12	5	738	727
10-12	5	416	362
11-12	5	1110	1115
13-12	5	365	330
14-12	5	296	296
-21-11	5	435	413
-20-11	5	439	410
-19-11	5	341	396
10-11	5	667	663
11-11	5	396	333
12-11	5	283	298
15-11	5	432	390
16-11	5	387	295
-19-10	5	257	199
-18-10	5	308	261
-16-10	5	602	627

H K	L	FOBS	FCALC
-15-10	5	451	485
10-10	5	1345	1280
12-10	5	965	951
16-10	5	294	310
-20 -9	5	601	686
-19 -9	5	295	293
-17 -9	5	362	397
-16 -9	5	399	475
15 -9	5	284	237
16 -9	5	616	648
-18 -8	5	583	626
-17 -8	5	315	344
11 -8	5	1348	1372
12 -8	5	321	289
13 -8	5	379	349
14 -8	5	386	365
16 -8	5	300	237
-21 -7	5	408	403
-19 -7	5	319	346
-18 -7	5	414	403
12 -7	5	700	679
14 -7	5	689	710
17 -7	5	316	416
-19 -6	5	463	457
-18 -6	5	688	699
-17 -6	5	541	549
13 -6	5	335	415
14 -6	5	544	533
15 -6	5	529	517
-17 -5	5	908	947
12 -5	5	270	203
13 -5	5	1185	1247
15 -5	5	357	401
-21 -4	5	366	332
-19 -4	5	582	613
-18 -4	5	359	398
15 -4	5	634	641
-21 -3	5	461	498
-19 -3	5	458	485
-18 -3	5	273	271
13 -3	5	285	282
14 -3	5	746	813
17 -3	5	520	593
-22 -2	5	304	337
-19 -2	5	309	352
-18 -2	5	587	560
13 -2	5	330	294

H K	L	FOBS	FCALC
14 -2	5	415	400
-22 -1	5	367	320
-21 -1	5	414	415
-20 -1	5	837	823
-19 -1	5	538	559
15 -1	5	460	507
16 -1	5	648	696
17 -1	5	443	494
18 -1	5	435	481
-20 0	5	261	171
-18 0	5	741	756
14 0	5	270	320
16 0	5	294	403
-5-24	6	389	372
-3-24	6	285	254
-1-24	6	267	238
-7-23	6	321	343
-5-23	6	259	219
-4-23	6	372	317
-2-23	6	327	326
0-23	6	252	248
1-23	6	292	288
-9-22	6	501	462
-7-22	6	250	283
-6-22	6	342	270
-4-22	6	266	240
-1-22	6	394	334
2-22	6	258	255
3-22	6	493	461
5-22	6	400	377
-6-21	6	282	285
-3-21	6	705	662
-2-21	6	309	251
-1-21	6	477	457
6-21	6	299	194
-14-20	6	301	216
-10-20	6	365	351
-9-20	6	388	410
-8-20	6	522	545
-7-20	6	297	303
-6-20	6	250	203
-2-20	6	286	290
0-20	6	298	273
2-20	6	412	457
3-20	6	383	336
4-20	6	675	668
5-20	6	342	301

H K	L	FOBS	FCALC
-14-19	6	478	480
-11-19	6	359	400
-8-19	6	270	271
-6-19	6	336	314
-4-19	6	563	552
-2-19	6	836	802
1-19	6	358	348
8-19	6	317	276
-12-18	6	391	384
-10-18	6	243	300
-9-18	6	468	463
-8-18	6	596	607
-7-18	6	466	455
-5-18	6	351	332
-4-18	6	556	540
0-18	6	551	541
1-18	6	304	363
3-18	6	588	587
4-18	6	508	517
5-18	6	523	[illegible]
8-18	6	401	392
-15-17	6	335	331
-13-17	6	441	391
-12-17	6	594	616
-10-17	6	738	767
-6-17	6	861	866
-4-17	6	440	410
-3-17	6	472	519
-1-17	6	222	246
0-17	6	624	657
2-17	6	951	985
6-17	6	483	490
8-17	6	298	304
9-17	6	376	374
11-17	6	368	306
-18-16	6	350	330
-16-16	6	256	314
-14-16	6	276	286
-13-16	6	422	437
-12-16	6	527	547
-10-16	6	243	296
-9-16	6	323	383
2-16	6	554	557
4-16	6	288	277
6-16	6	516	506
7-16	6	384	346
8-16	6	510	477

H K	L	FOBS	FCALC
12-16	6	390	352
-19-15	6	305	320
-13-15	6	281	292
-12-15	6	290	225
-11-15	6	1002	1067
-10-15	6	262	205
5-15	6	301	283
6-15	6	[illegible]	419
7-15	6	602	596
13-15	6	392	423
-17-14	6	475	494
-13-14	6	727	753
-12-14	6	242	218
6-14	6	427	408
7-14	6	882	866
9-14	6	523	563
11-14	6	309	256
13-14	6	450	448
-19-13	6	298	316
-16-13	6	268	230
-15-13	6	478	465
-14-13	6	280	298
7-13	6	361	346
8-13	6	359	391
9-13	6	437	387
10-13	6	301	331
11-13	6	411	397
12-13	6	488	455
13-13	6	279	294
14-13	6	295	291
-19-12	6	333	293
-16-12	6	250	271
-14-12	6	283	220
8-12	6	698	700
12-12	6	336	329
-16-11	6	361	400
-15-11	6	562	1022
-14-11	6	506	552
9-11	6	865	901
10-11	6	765	757
11-11	6	668	708
-20-10	6	588	621
-17-10	6	235	199
-20 -9	6	314	319
-18 -9	6	275	249
-16 -9	6	817	832
10 -9	6	1079	1107

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
11	-9	6	438	435	13	-2	6	301	286	-10	-18	7	330	258	4	-14	7	277	293	-21	-7	7	392	380
12	-9	6	398	346	15	-2	6	663	758	-9	-18	7	238	303	5	-14	7	730	724	-18	-7	7	864	839
-22	-9	6	303	262	16	-2	6	297	244	-6	-18	7	380	394	7	-14	7	428	463	-16	-7	7	384	382
-21	-8	6	464	502	17	-2	6	427	510	-5	-18	7	227	216	10	-14	7	272	371	11	-7	7	266	219
-20	-8	6	307	260	-21	-1	6	288	212	-4	-18	7	384	387	11	-14	7	306	218	12	-7	7	484	508
-19	-8	6	472	471	-20	-1	6	439	439	-3	-18	7	536	508	12	-14	7	319	279	15	-7	7	433	506
-18	-8	6	434	435	12	-1	6	454	521	-2	-18	7	359	384	-18	-13	7	429	343	-22	-6	7	293	245
-17	-8	6	260	249	14	-1	6	341	325	-1	-18	7	429	400	-17	-13	7	260	214	-19	-6	7	302	276
-16	-8	6	508	544	-22	0	6	727	700	0	-18	7	356	353	-16	-13	7	256	291	-17	-6	7	238	240
10	-8	6	426	434	-20	0	6	650	661	1	-18	7	415	447	-15	-13	7	267	275	12	-6	7	411	464
12	-8	6	440	433	14	0	6	625	616	2	-18	7	440	490	-13	-13	7	469	487	13	-6	7	782	759
15	-8	6	461	506	16	0	6	849	868	3	-18	7	299	236	3	-13	7	710	644	14	-6	7	440	440
16	-8	6	294	291	-8	-23	7	277	247	6	-18	7	286	228	7	-13	7	611	599	-19	-5	7	619	567
-22	-7	6	310	264	-6	-23	7	322	230	9	-18	7	391	376	8	-13	7	478	466	-17	-5	7	948	971
-19	-7	6	319	304	-5	-23	7	287	287	-16	-17	7	296	268	11	-13	7	410	359	11	-5	7	405	538
-18	-7	6	501	596	-1	-23	7	305	317	-12	-17	7	245	221	-15	-12	7	744	777	13	-5	7	329	305
11	-7	6	513	542	-7	-22	7	384	360	-10	-17	7	266	262	6	-12	7	440	424	-19	-4	7	333	333
12	-7	6	413	432	-3	-22	7	494	493	-9	-17	7	472	484	9	-12	7	771	799	-17	-4	7	208	281
14	-7	6	600	591	-2	-22	7	250	182	-7	-17	7	474	486	11	-12	7	448	448	10	-4	7	455	504
-21	-6	6	326	237	-9	-21	7	514	483	-6	-17	7	766	756	12	-12	7	363	375	12	-4	7	936	610
-18	-6	6	549	542	-7	-21	7	258	225	-4	-17	7	736	702	-21	-11	7	311	328	13	-4	7	781	755
-17	-6	6	692	735	-3	-21	7	268	263	-1	-17	7	359	347	-15	-11	7	425	384	14	-4	7	314	351
11	-6	6	387	419	-2	-21	7	300	265	0	-17	7	507	535	-14	-11	7	439	428	15	-4	7	351	337
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13	-6	6	469	545	0	-21	7	271	236	5	-17	7	286	286	-20	-10	7	417	417	-20	-3	7	254	255
14	-6	6	471	482	3	-21	7	642	649	6	-17	7	513	538	-17	-10	7	255	291	-18	-3	7	569	573
-19	-5	6	525	501	5	-21	7	433	376	8	-17	7	472	447	-16	-10	7	753	791	-17	-3	7	420	420
-17	-5	6	457	504	-8	-20	7	474	439	-12	-16	7	719	725	-15	-10	7	340	417	11	-3	7	608	627
13	-5	6	827	848	-4	-20	7	482	488	-11	-16	7	452	468	8	-10	7	838	835	12	-3	7	393	411
15	-5	6	492	546	-3	-20	7	396	353	-10	-16	7	546	532	10	-10	7	1003	1000	15	-3	7	412	371
17	-5	6	302	254	-2	-20	7	418	421	-8	-16	7	253	282	-22	-9	7	466	432	-21	-2	7	416	389
-20	-4	6	285	205	4	-20	7	363	345	-7	-16	7	563	564	-20	-9	7	345	326	-20	-2	7	370	370
-18	-4	6	355	312	6	-20	7	287	213	-6	-16	7	538	522	-19	-9	7	328	333	-19	-2	7	447	431
-17	-4	6	813	809	-14	-19	7	326	286	0	-16	7	863	847	-17	-9	7	254	289	11	-2	7	733	761
12	-4	6	368	350	-10	-19	7	576	584	1	-16	7	700	798	8	-9	7	276	256	12	-2	7	338	340
13	-4	6	656	740	-8	-19	7	552	539	2	-16	7	678	711	10	-9	7	318	316	14	-2	7	394	463
14	-4	6	285	352	-5	-19	7	323	314	6	-16	7	403	468	13	-9	7	285	219	-22	-1	7	512	525
-22	-3	6	315	307	-3	-19	7	238	302	-17	-15	7	541	528	14	-9	7	519	491	-21	-1	7	308	315
-19	-3	6	503	486	-2	-19	7	545	515	-13	-15	7	459	472	15	-9	7	330	279	-18	-1	7	458	446
-18	-3	6	573	559	0	-19	7	277	202	4	-15	7	359	350	-20	-8	7	400	365	12	-1	7	254	275
12	-3	6	590	585	2	-19	7	541	508	5	-15	7	495	473	-17	-8	7	241	196	13	-1	7	315	283
14	-3	6	578	621	4	-19	7	699	653	7	-15	7	869	810	-16	-8	7	723	730	14	-1	7	404	448
15	-3	6	327	303	-16	-18	7	327	322	9	-15	7	290	239	9	-8	7	970	912	15	-1	7	400	438
-21	-2	6	567	559	-15	-18	7	260	249	-19	-14	7	290	301	10	-8	7	293	228	16	-1	7	471	488
-19	-2	6	360	369	-13	-18	7	328	361	-14	-14	7	238	182	11	-8	7	588	579	-20	0	7	740	708
-18	-2	6	554	549	-12	-18	7	299	324	-13	-14	7	516	509	12	-8	7	292	268	-18	0	7	261	192
12	-2	6	600	599	-11	-18	7	391	382	-11	-14	7	791	831	14	-8	7	333	361	-6	-22	8	275	226

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H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC
-3-22	8	350	332	4-16	8	356	370	5-11	8	411	410	9 -3	8	753	751	-8-17	9	354	371
-9-21	8	434	421	5-16	8	411	319	6-11	8	257	257	10 -3	8	348	376	-6-17	9	737	717
-7-21	8	246	226	6-16	8	644	675	8-11	8	393	348	12 -3	8	727	744	-5-17	9	359	296
-5-21	8	299	303	7-16	8	459	364	9-11	8	580	606	14 -3	8	506	497	-3-17	9	459	461
-3-21	8	356	381	8-16	8	432	379	10-11	8	332	304	-21 -2	8	335	296	3-17	9	249	175
-11-20	8	300	229	-14-15	8	294	228	-16-10	8	428	433	-18 -2	8	499	456	4-17	9	264	275
-10-20	8	352	346	-13-15	8	701	713	-15-10	8	300	293	-17 -2	8	252	299	6-17	9	498	517
-4-20	8	392	378	-12-15	8	254	277	-14-10	8	795	866	9 -2	8	730	701	-17-16	9	265	280
-2-20	8	570	560	-11-15	8	586	614	10-10	8	541	521	10 -2	8	305	270	-14-16	9	294	363
2-20	8	447	468	-9-15	8	246	295	-20 -9	8	452	428	11 -2	8	488	462	-13-16	9	251	215
3-20	8	350	354	-8-15	8	253	250	-18 -9	8	299	282	15 -2	8	406	387	-12-16	9	553	564
4-20	8	321	286	-7-15	8	496	503	-16 -9	8	804	812	-21 -1	8	304	311	-5-16	9	284	353
-13-19	8	309	206	-1-15	8	843	858	-15 -9	8	300	314	-20 -1	8	419	369	-4-16	9	236	215
-10-19	8	300	321	0-15	8	520	530	8 -9	8	676	688	-18 -1	8	343	335	-2-16	9	426	427
-8-19	8	502	557	1-15	8	991	986	9 -9	8	264	190	-17 -1	8	502	475	-1-16	9	368	334
-4-19	8	592	560	5-15	8	317	320	10 -9	8	455	537	9 -1	8	820	924	0-16	9	760	703
-2-19	8	357	299	-19-14	8	449	414	-18 -8	8	528	517	10 -1	8	568	623	1-16	9	243	189
4-19	8	532	515	-17-14	8	396	354	-17 -8	8	322	303	11 -1	8	341	372	2-16	9	302	204
-10-18	8	397	469	-11-14	8	406	388	-15 -8	8	320	324	-22 0	8	583	575	6-16	9	291	70
-9-18	8	257	258	-9-14	8	232	194	7 -8	8	516	591	10 0	8	823	843	-11-15	9	339	381
-7-18	8	312	357	2-14	8	379	387	8 -8	8	362	395	14 0	8	406	421	-8-15	9	410	408
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H3DEP+ RE2(CO)6CL3-   MO DATA   40-55 DEG 2THETA   10 FO AND 10FC   PAGE 8

H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC	H K	L	FOBS	FCALC
3-13	9	246	264	-22 -7	9	302	103	-2-20	10	326	314	-2-14	10	390	327	10-10	10	456	444
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-11-12	9	438	472	10 -6	9	321	313	-3-18	10	368	359	-11-13	10	292	302	-15 -8	10	512	508
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H3OEP+ RE2(CO)6CL3- MO DATA 40-55 DEG 2THETA 10 FO AND 10FC

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5	-14	11	343	328	-8	-10	11	233	160	-19	-4	11	406	368	-7	-15	12	550	507	-10	-9	12	564	580

H3OEP+ RE2(CO)6CL3- MO DATA 40-55 DEG 2THETA 10 FO AND 10FC

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-4	-9	12	226	213	5	-5	12	617	561	-3	-14	13	251	262	-5	-8	13	319	300	-17	-3	13	310	294
0	-9	12	600	602	7	-5	12	344	333	-15	-13	13	295	208	-3	-8	13	247	247	-16	-3	13	273	262
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2	-9	12	677	704	-15	-4	12	390	351	-13	-13	13	285	262	1	-8	13	563	502	-13	-3	13	372	293
3	-9	12	301	330	-14	-4	12	426	333	-12	-13	13	249	242	3	-8	13	405	349	-12	-3	13	248	274
-17	-8	12	285	332	-13	-4	12	877	847	-11	-13	13	250	160	4	-8	13	374	290	-11	-3	13	267	318
-15	-8	12	321	311	-12	-4	12	383	354	-9	-13	13	266	252	-14	-7	13	537	479	-10	-3	13	241	165
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-3	-8	12	580	600	-18	-3	12	276	217	-11	-12	13	359	359	-15	-6	13	265	279	-16	-2	13	277	257
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-1	-8	12	271	211	-14	-3	12	297	293	-5	-12	13	260	268	-9	-6	13	423	363	-12	-2	13	372	350
0	-8	12	338	368	1	-3	12	615	593	-3	-12	13	311	323	-8	-6	13	724	746	-11	-2	13	529	480
4	-8	12	324	309	3	-3	12	462	481	1	-12	13	539	471	-7	-6	13	577	532	-9	-2	13	228	226
5	-8	12	272	256	4	-3	12	428	423	-11	-11	13	236	241	-6	-6	13	552	543	-8	-2	13	746	695
7	-8	12	392	416	6	-3	12	435	391	-10	-11	13	308	280	-3	-6	13	237	235	-5	-2	13	347	357
8	-8	12	287	208	-17	-2	12	479	425	-6	-11	13	301	380	1	-6	13	304	325	-4	-2	13	244	264
-20	-7	12	349	340	-15	-2	12	335	323	-5	-11	13	449	465	2	-6	13	293	229	-2	-2	13	232	166
-18	-7	12	289	252	-14	-2	12	527	490	-4	-11	13	318	308	3	-6	13	269	216	-1	-2	13	428	486
-11	-7	12	534	539	3	-2	12	370	304	-3	-11	13	322	291	4	-6	13	498	431	1	-2	13	606	689
-9	-7	12	331	295	4	-2	12	516	521	0	-11	13	258	178	5	-6	13	385	346	3	-2	13	307	275
-3	-7	12	360	370	7	-2	12	490	553	-16	-10	13	369	343	6	-6	13	365	307	4	-2	13	308	319
-2	-7	12	342	407	9	-2	12	423	372	-12	-10	13	458	444	-15	-5	13	612	583	6	-2	13	291	262
-1	-7	12	276	234	-20	-1	12	290	239	-10	-10	13	297	293	-13	-5	13	665	618	-18	-1	13	379	352
1	-7	12	531	517	-14	-1	12	263	167	-4	-10	13	496	473	-9	-5	13	407	429	-17	-1	13	309	285
4	-7	12	273	294	-13	-1	12	345	291	0	-10	13	617	599	-5	-5	13	269	289	-14	-1	13	300	259
6	-7	12	474	449	1	-1	12	554	605	2	-10	13	557	531	-3	-5	13	479	465	-11	-1	13	308	215
-15	-6	12	312	203	2	-1	12	912	948	-18	-9	13	373	293	-1	-5	13	952	934	-10	-1	13	548	517
-14	-6	12	517	512	3	-1	12	432	420	-10	-9	13	291	336	3	-5	13	363	326	-4	-1	13	502	540
-13	-6	12	645	641	10	-1	12	303	213	-6	-9	13	569	576	-19	-4	13	326	316	-3	-1	13	473	471
-12	-6	12	303	298	-18	0	12	515	455	-5	-9	13	301	263	-15	-4	13	280	287	-1	-1	13	299	218
-11	-6	12	312	319	-16	0	12	602	542	-4	-9	13	476	475	-13	-4	13	349	296	1	-1	13	427	405
-10	-6	12	233	247	2	0	12	476	460	-3	-9	13	299	282	-11	-4	13	261	263	2	-1	13	548	504
-1	-6	12	607	553	4	0	12	395	359	2	-9	13	371	344	-10	-4	13	257	239	3	-1	13	285	281
0	-6	12	554	584	6	0	12	506	490	6	-9	13	363	382	-9	-4	13	775	727	4	-1	13	297	229
3	-6	12	319	296	8	0	12	669	694	-16	-8	13	300	282	-8	-4	13	393	358	6	-1	13	335	346
4	-6	12	491	525	-8	-16	13	341	321	-12	-8	13	254	258	-7	-4	13	949	937	8	-1	13	309	343
5	-6	12	295	247	-13	-15	13	380	387	-11	-8	13	379	360	-6	-4	13	414	366	-16	0	13	484	450
6	-6	12	336	338	-3	-15	13	348	329	-9	-8	13	228	254	-3	-4	13	462	473	-12	0	13	583	542
-19	-5	12	502	470	-1	-15	13	464	407	-8	-9	13	550	532	1	-4	13	347	303	-10	0	13	402	412
-15	-5	12	432	399	-9	-14	13	318	292	-7	-8	13	307	314	4	-4	13	294	269	-4	0	13	311	263

H3DEF+ RE2(CO)6CL3- MO DATA 40-55 DEG 2THETA 10 FO AND 10FC

H	K	L	FOBS	FCALC
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8	0	13	317	262
-9	-15	14	264	283
-7	-15	14	309	293
-13	-14	14	269	192
-3	-14	14	442	386
-1	-14	14	343	306
-9	-13	14	293	275
-14	-12	14	270	258
-11	-12	14	360	322
-7	-12	14	283	204
-2	-12	14	292	284
0	-12	14	258	144
1	-12	14	312	262
-12	-11	14	270	272
-5	-11	14	324	348
-4	-11	14	408	350
0	-11	14	327	322
-12	-10	14	262	243
-10	-10	14	435	409
-6	-10	14	420	427
0	-10	14	271	232
2	-10	14	404	338
-16	-9	14	303	268
-12	-9	14	409	381
-6	-9	14	281	232
-4	-9	14	262	237
0	-9	14	355	376
-14	-8	14	328	293
-11	-8	14	288	291
-6	-8	14	303	329
-3	-8	14	223	156
-2	-8	14	351	308
-1	-8	14	282	207
-13	-7	14	252	244
-11	-7	14	323	284
-10	-7	14	286	337
-8	-7	14	659	669
-6	-7	14	270	257
-5	-7	14	252	245
-1	-7	14	358	352
1	-7	14	321	330
4	-7	14	474	402
-15	-6	14	426	396
-14	-6	14	332	338
-13	-6	14	345	316

H	K	L	FOBS	FCALC
-7	-6	14	323	293
-6	-6	14	228	193
-3	-6	14	527	524
-2	-6	14	381	361
-1	-6	14	313	250
0	-6	14	255	249
-13	-5	14	294	251
-9	-5	14	752	730
-8	-5	14	262	224
-7	-5	14	672	654
-1	-5	14	268	158
3	-5	14	473	397
5	-5	14	393	384
-15	-4	14	510	443
-14	-4	14	399	379
-13	-4	14	396	350
-11	-4	14	245	230
-7	-4	14	427	433
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-4	-4	14	305	286
-3	-4	14	403	380
-2	-4	14	362	346
-1	-4	14	502	490
0	-4	14	284	251
-17	-3	14	399	322
-10	-3	14	326	329
-9	-3	14	313	262
-8	-3	14	658	644
-7	-3	14	251	242
-6	-3	14	445	330
-5	-3	14	343	298
-3	-3	14	243	235
-1	-3	14	280	257
4	-3	14	471	381
-14	-2	14	331	313
-13	-2	14	297	240
-11	-2	14	402	356
-7	-2	14	370	352
-6	-2	14	379	391
-5	-2	14	459	450
-2	-2	14	367	382
1	-2	14	409	379
5	-2	14	332	238
-18	-1	14	303	222
-16	-1	14	315	290
-12	-1	14	314	259
-9	-1	14	272	210

H	K	L	FOBS	FCALC
-5	-1	14	423	405
-4	-1	14	545	493
0	-1	14	410	428
-14	0	14	312	301
-12	0	14	438	350
-10	0	14	391	339
-6	0	14	730	729
0	0	14	414	290
2	0	14	617	543
6	0	14	457	465
-5	-12	15	324	281
-12	-11	15	298	253
-11	-11	15	271	217
-6	-10	15	264	296
-5	-10	15	260	206
-4	-10	15	247	258
0	-10	15	341	311
-10	-9	15	266	231
0	-9	15	369	330
-10	-8	15	274	216
-5	-8	15	272	192
-16	-7	15	283	243
-14	-7	15	330	308
-8	-7	15	299	264
-4	-7	15	297	306
-2	-7	15	502	444
-9	-6	15	462	419
-8	-6	15	368	341
-1	-6	15	353	317
-15	-5	15	464	420
-13	-5	15	269	228
-7	-5	15	371	347
-3	-5	15	589	576
-1	-5	15	395	371
-11	-4	15	255	122
-9	-4	15	578	580
-8	-4	15	301	274
-1	-4	15	270	240
3	-4	15	361	303
-15	-3	15	297	288
-14	-3	15	264	256
-11	-3	15	378	344
-8	-3	15	287	212
-7	-3	15	368	339
-4	-3	15	250	242
-2	-3	15	461	480
0	-3	15	312	261

H	K	L	FOBS	FCALC
1	-3	15	292	242
-17	-2	15	358	320
-12	-2	15	248	163
-10	-2	15	348	362
-8	-2	15	376	374
-7	-2	15	383	329
-5	-2	15	458	443
-12	-1	15	308	262
-10	-1	15	305	276
-8	-1	15	349	320
-6	-1	15	289	259
-1	-1	15	308	312
0	-1	15	316	286
1	-1	15	310	246
2	-1	15	312	293
-18	0	15	436	360
-16	0	15	336	310
-6	0	15	512	463
-4	0	15	324	400
-12	-10	16	336	322
-6	-9	16	248	307
-13	-8	16	254	204
-11	-8	16	287	203
-9	-6	16	255	196
-4	-6	16	323	234
-3	-6	16	270	237
-2	-6	16	295	271
-11	-5	16	257	259
-9	-5	16	374	416
-3	-5	16	283	235
-15	-4	16	275	261
-7	-4	16	268	335
-3	-4	16	307	331
-10	-3	16	284	287
-8	-3	16	315	314
-4	-3	16	262	209
-8	-2	16	275	235
-7	-1	16	280	271
-6	-1	16	414	362
-12	0	16	306	243
-4	0	16	308	234
0	0	16	349	335
-9	-5	17	325	266
-11	-4	17	277	257
-3	-4	17	252	248
-12	-1	17	300	244

H	K	L	FOBS	FCALC

ATOM	X	Y	Z	U(11)	U(22)	U(33)	U(12)	U(13)	U(23)
RE(1)	0.12959(1)	0.19521(1)	0.16057(2)	435(1)	517(1)	626(1)	-46(3)	299(2)	-21(3)
RE(2)	0.29168(2)	0.09642(1)	0.21983(2)	486(1)	524(1)	542(1)	21(3)	165(2)	-99(3)
CL(1)	0.2643(1)	0.2022(1)	0.3048(1)	51(1)	52(1)	57(1)	-17(1)	22(1)	-21(1)
CL(2)	0.1539(1)	0.0741(1)	0.2135(1)	56(1)	49(1)	61(1)	-19(1)	31(1)	-6(1)
CL(3)	0.2143(1)	0.1635(1)	0.0594(1)	56(1)	64(1)	52(1)	2(2)	35(1)	-2(2)
N(1)	0.2253(3)	0.0536(3)	0.6760(5)	37(3)	69(4)	60(4)	17(6)	-13(6)	-14(7)
N(2)	0.0901(3)	0.1398(3)	0.5997(4)	42(3)	85(4)	39(3)	15(6)	29(4)	-13(6)
N(3)	0.0159(3)	0.0529(3)	0.4024(4)	38(3)	64(4)	40(3)	-8(6)	5(5)	-7(6)
N(4)	0.1633(3)	-0.0275(3)	0.4853(5)	48(3)	43(3)	63(4)	9(6)	0(6)	-4(6)
C(1)	0.2888(4)	0.0103(4)	0.6951(6)	38(4)	63(5)	60(5)	18(8)	-8(7)	-7(8)
C(2)	0.3458(4)	0.0300(4)	0.7918(6)	32(3)	61(5)	65(5)	3(7)	4(7)	7(8)
C(3)	0.3164(4)	0.0831(4)	0.8307(6)	37(3)	56(4)	46(4)	-20(7)	-2(6)	-18(7)
C(4)	0.2412(4)	0.0993(4)	0.7552(6)	52(4)	69(5)	49(4)	6(8)	24(6)	-4(8)
C(5)	0.1803(4)	0.1490(4)	0.7598(6)	47(4)	75(5)	43(4)	12(8)	10(6)	-17(8)
C(6)	0.1155(4)	0.1678(4)	0.6889(6)	45(4)	76(5)	49(4)	28(8)	24(6)	-6(8)
C(7)	0.0603(4)	0.2144(4)	0.7029(6)	53(4)	78(5)	46(4)	33(8)	34(6)	-21(8)
C(8)	-0.0033(4)	0.2174(4)	0.6121(6)	47(4)	68(5)	57(4)	22(8)	30(6)	-10(8)
C(9)	0.0065(4)	0.1702(4)	0.5404(5)	35(3)	80(5)	49(4)	27(7)	26(6)	13(8)
C(10)	-0.0467(4)	0.1512(4)	0.4424(6)	34(3)	71(5)	44(4)	25(7)	10(6)	0(8)
C(11)	-0.0437(4)	0.0993(4)	0.3796(6)	35(3)	60(4)	52(4)	13(7)	30(6)	4(8)
C(12)	-0.1003(4)	0.0803(4)	0.2782(5)	34(3)	67(5)	44(4)	1(7)	15(6)	0(7)
C(13)	-0.0739(4)	0.0248(4)	0.2442(5)	34(3)	55(4)	46(3)	-10(7)	16(5)	4(7)
C(14)	0.0315(4)	0.0073(3)	0.3225(5)	38(3)	48(4)	45(3)	0(7)	14(6)	0(7)
C(15)	0.0533(4)	-0.0445(4)	0.3189(6)	48(4)	48(4)	51(4)	-13(7)	11(7)	1(7)
C(16)	0.1273(4)	-0.0607(3)	0.3919(6)	48(4)	42(4)	62(4)	0(7)	17(7)	-3(7)
C(17)	0.1763(5)	-0.1138(4)	0.3800(7)	52(4)	57(4)	73(5)	39(8)	-10(8)	-29(9)
C(18)	0.2404(5)	-0.1143(4)	0.4655(8)	65(5)	66(5)	111(7)	71(9)	-52(11)	-57(10)
C(19)	0.2328(5)	-0.0611(4)	0.5347(7)	60(5)	63(5)	78(6)	33(9)	-6(9)	-29(9)
C(20)	0.2916(5)	-0.0423(4)	0.6316(7)	49(4)	76(5)	91(6)	54(8)	-19(9)	-25(10)
C(21)	0.4271(5)	-0.0013(5)	0.8404(7)	52(5)	74(6)	90(5)	13(10)	-21(9)	-22(11)
C(22)	0.4863(6)	0.0320(7)	0.8082(13)	50(5)	110(9)	256(15)	28(13)	58(15)	-1(22)
C(23)	0.3573(5)	0.1192(5)	0.9336(7)	62(5)	97(7)	65(5)	41(10)	28(8)	7(10)
C(24)	0.3916(7)	0.1944(6)	0.9233(10)	89(8)	102(8)	115(9)	-36(14)	-17(15)	-24(15)
C(25)	0.0749(5)	0.2522(5)	0.8054(7)	55(5)	86(6)	75(5)	15(10)	22(8)	4(11)
C(26)	0.1235(6)	0.3095(6)	0.8207(9)	92(7)	92(7)	118(8)	11(13)	37(13)	-53(13)
C(27)	-0.0751(5)	0.2625(5)	0.5872(7)	61(5)	80(6)	68(5)	27(9)	24(8)	-24(9)
C(28)	-0.0636(7)	0.3295(6)	0.5443(9)	91(7)	102(7)	102(9)	69(13)	-12(14)	9(14)
C(29)	-0.1749(4)	0.1205(5)	0.2196(6)	33(3)	95(6)	60(4)	24(8)	7(7)	-29(9)
C(30)	-0.1544(5)	0.1702(5)	0.1441(8)	67(5)	90(6)	90(6)	74(10)	38(9)	57(11)
C(31)	-0.1094(4)	-0.0116(4)	0.1401(6)	41(4)	63(5)	63(4)	-15(8)	8(7)	1(9)
C(32)	-0.0744(5)	0.0068(5)	0.0620(6)	83(5)	82(6)	61(5)	-38(10)	37(8)	-43(10)
C(33)	0.1596(5)	-0.1551(4)	0.2825(8)	61(5)	63(5)	83(6)	20(9)	-7(10)	-23(10)
C(34)	0.1841(6)	-0.1190(5)	0.2052(8)	64(6)	89(6)	103(7)	23(11)	3(11)	-66(12)
C(35)	0.3073(8)	-0.1776(8)	0.5156(9)	163(10)	217(13)	91(7)	-190(19)	58(14)	-39(18)
C(36)	0.3570(10)	-0.1500(7)	0.4839(11)	246(15)	115(11)	134(9)	4(22)	170(17)	17(17)
C(37)	0.0347(4)	0.1783(4)	0.0446(6)	54(4)	67(5)	70(5)	-3(8)	31(7)	14(9)
C(38)	0.0735(5)	0.2119(4)	0.2474(7)	95(6)	53(5)	69(5)	-59(9)	29(9)	-1(9)
C(39)	0.1205(4)	0.2866(4)	0.1224(7)	45(3)	68(5)	103(5)	25(8)	62(7)	-7(9)
C(40)	0.2942(5)	0.1217(4)	0.2252(7)	55(5)	60(5)	98(6)	9(9)	22(9)	-34(10)
C(41)	0.2964(4)	0.0301(4)	0.1386(7)	49(4)	59(5)	83(5)	-11(8)	7(8)	-28(9)
C(42)	0.3400(6)	0.3459(4)	0.3435(8)	75(6)	56(5)	89(6)	-14(10)	8(10)	-9(10)
O(1)	-0.0213(3)	0.1670(3)	-0.0272(6)	61(4)	107(5)	107(5)	-34(8)	-36(8)	18(9)
O(2)	0.0356(3)	0.2237(3)	0.3005(5)	103(3)	108(5)	118(4)	3(7)	142(5)	-5(8)
O(3)	0.1156(4)	0.3419(3)	0.0987(5)	103(4)	53(3)	154(5)	32(7)	87(8)	25(8)
O(4)	0.4561(3)	0.1377(4)	0.2273(6)	56(3)	113(5)	163(6)	-44(7)	69(7)	-54(10)
O(5)	0.2393(3)	-0.0237(3)	0.0877(5)	85(4)	73(4)	121(4)	1(7)	52(6)	-52(7)
O(6)	0.3703(5)	0.0150(4)	0.4191(6)	140(7)	99(5)	104(5)	25(11)	-36(10)	61(9)
O(7)	0.1883(3)	0.1236(3)	0.4706(4)	79(3)	79(4)	81(3)	-2(6)	73(5)	0(6)
H(1)	0.193 (3)	0.049 (3)	0.642 (4)	40					
H(2)	0.100 (3)	0.140 (3)	0.544 (4)	40					
H(3)	0.046 (3)	0.052 (3)	0.445 (4)	40					

APPENDIX

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